STIC Search Report
EIC 1700

STIC Database Tracking Number: 214288

TO:	From:
Ben Sackey Location: REM 5B31 Art Unit : 1624 February 7, 2007 Case Serial Number: 10/802541	Kathleen Fuller Location: EIC 1700 REMSEN 4B28 Phone: 571/272-2505 Kathleen.Fuller@uspto.gov

Search Notes

ACCESS DB # 214288

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Mrs Fuller

Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: Ben Sackey Examiner #: 23489 Date: 01/25/07

Art Unit: 1624 Phone Number: 2-0704 Serial Number: 10/802,541

Location (Bldg/Room#): Rem 5B31 (Mailbox #): _____ Results Format Preferred (circle): ~~PAPER~~ DISK

****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Process for prep. 4-(1H-1,2,4-triazol-1-ylmethyl benzonitril

Inventors (please provide full names): Wadhwa et al.

SCIENTIFIC REFERENCE B
Sci & Tech In

JAN 30

Earliest Priority Date: _____

Pat. & T.M. Office

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

A process for preparing 4-(1H-1,2,4-triazol-1-ylmethyl)benzonitri
of formula (2), comprising reacting a salt of 1,2,4-triazol
of formula (ii) in the presence of a solvent at between
25-30°C, adding a salt of α-halo substituted
tolunitrile of formula (3) in a solvent at 10°C, adding
demineralized H_2O and extracting into dichloromethane and
crystallizing the product.

Thanks

=> FILE CASRE
FILE 'CASREACT' ENTERED AT 11:50:04 ON 07 FEB 2007

FILE CONTENT:1840 - 4 Feb 2007 VOL 146 ISS 6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

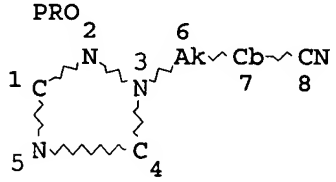
****
*
* CASREACT now has more than 10 million reactions *
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> D QUE
L48 STR

This as a product



NODE ATTRIBUTES:
CONNECT IS E2 RC AT 6
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 7
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 8

5 CA references

STEREO ATTRIBUTES: NONE
L50 5 SEA FILE=CASREACT SSS FUL L48 (13 REACTIONS)

=> D BIB ABS FHIT 1-5

L50 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

✓ applicant

AN 143:306322 CASREACT
TI Condensation process for producing 4-[(1H-1,2,4-triazol-1-yl)methyl]benzonitrile from an alkali metal salt of 1,2,4-triazole and a 4-(halomethyl)benzonitrile

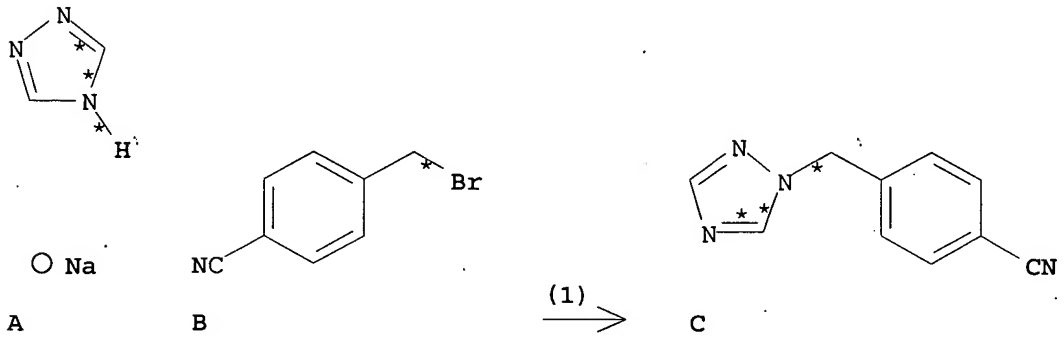
IN Wadhwa, Lalit Kumar; Saxena, Rahul
PA India
SO U.S. Pat. Appl. Publ., 4 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005209294	A1	20050922	US 2004-802541	20040317

PRAI US 2004-802541 20040317

AB A process for producing 4-[(1H-1,2,4-triazol-1-yl)methyl]benzonitrile comprises reacting an alkali metal salt of 1,2,4-triazole (e.g., the sodium salt) with a 4-(halomethyl)benzonitrile [e.g., 4-(bromomethyl)benzonitrile] in the presence of DMF, adding water, extracting the mixture with dichloromethane, and distilling off the organic solvent.

RX(1) OF 1 A + B ===> C



A B C

RX(1) RCT A 41253-21-8, B 17201-43-3

STAGE(1)
SOL 68-12-2 DMF
CON SUBSTAGE(1) 25 - 30 deg C
SUBSTAGE(2) 30 minutes, 10 deg C
SUBSTAGE(3) 2 hours, 10 - 15 deg C

STAGE(2)
RGT D 7732-18-5 Water

PRO C **112809-25-3**

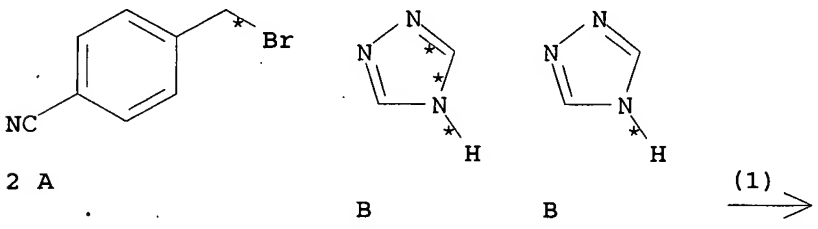
L50 ANSWER 2 OF 5 CASREACT COPYRIGHT 2007 ACS on STN
AN 142:482047 CASREACT
TI A precipitation method for the separation of the letrozole precursor 4-[1-(1,2,4-triazolyl)methyl]benzonitrile from its 4-[1-(1,3,4-triazolyl)methyl]benzonitrile byproduct isomer
IN Amala, Kompella; Rachakonda, Sreenivas; Adibhatla, Kalisatya Bhujangarao; Venkaiah Chowdary, Nannapaneni
PA Natco Pharma Limited, India
SO PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DT Patent

LA English
FAN.CNT 1

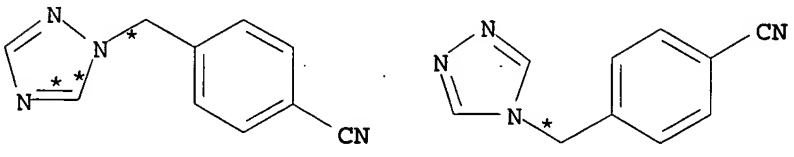
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005047269	A1	20050526	WO 2003-IN357	20031114
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2003282380	A1	20040606	AU 2003-282380	20031114
PRAI	WO 2003-IN357		20031114		

AB Separation of the letrozole precursor 4-[1-(1,2,4-triazolyl)methyl]benzonitrile from the unwanted byproduct 4-[1-(1,3,4-triazolyl)methyl]benzonitrile, both formed by the condensation reaction of 4-(bromomethyl)benzonitrile with 1,2,4-triazole, is achieved by: (A) dissolving the resultant crude isomeric mixture in dichloromethane or chloroform; (B) adding 10-14% iso-Pr alc. and hydrochloric acid to the resulting solution; (C) adding diisopropyl ether to precipitate the undesired 4-[1-(1,3,4-triazolyl)methyl]benzonitrile isomer as its hydrochloride; (D) filtering off the undesired isomer hydrochloride; (E) distilling off the filtrate completely; (F) adding dilute aqueous sodium hydroxide solution and dichloromethane to the residue to liberate the required 4-[1-(1,2,4-triazolyl)methyl]benzonitrile isomer as its free base; (G) evaporating the separated dichloromethane layer and charging hexane or petroleum ether; and (H) centrifuging the resultant 4-[1-(1,2,4-triazolyl)methyl]benzonitrile product and washing with hexane or petroleum ether.

RX(1) OF 1 2 A + 2 B ===> C + D



2 A B B



C D

RX(1) RCT A 17201-43-3, B 288-88-0

RGT E 584-08-7 K2CO3
PRO C 112809-25-3, D 112809-27-5
CAT 7681-11-0 KI
SOL 67-64-1 Me2CO
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 8 hours, 55 deg C
SUBSTAGE(3) 55 deg C -> room temperature
NTE other product also detected, regioselective, product ratio = 87:11:2, industrial manufacture
RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

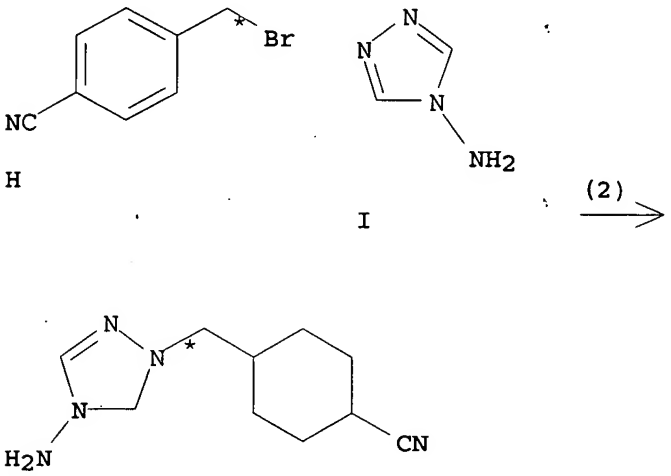
L50 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN
AN 141:225518 CASREACT
TI Improved regiospecific process for preparation of 4,4'-(1H-1,2,4-triazol-1-ylmethylene)bisbenzonitrile (Letrazole) free of isomeric impurities and 4,4',4''-methylidynetris(benzonitrile)
IN Patel, Hetalkumar Virendrabhai; Jani, Raja Jyotir; Thennati, Rajamannar
PA Sun Pharmaceutical Industries Limited, India
SO PCT Int. Appl., 15 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004076409	A2	20040910	WO 2004-IN36	20040205
	WO 2004076409	A3	20041104		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	IN 2003MU00167	A	20050204	IN 2003-MU167	20030206
	CA 2515181	A1	20040910	CA 2004-2515181	20040205
	EP 1594850	A2	20051116	EP 2004-708435	20040205
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	US 2006128775	A1	20060615	US 2005-544460	20050804
PRAI	IN 2003-MU167	20030206			
	WO 2004-IN36	20040205			

AB The title compound (1), useful as an antineoplastic agent (no data), is prepared by treating of 4-halomethylbenzonitrile, preferably 4-bromomethylbenzonitrile, with 4-amino-1,2,4-triazole in alc. solvent, preferably isopropanol, at 20-150° for 3-8 h to give 4-amino-1-[(4-cyanophenyl)methyl]-4H-1,2,4-triazolium halide (2), which is purified by washing with appropriate organic solvent and deaminated by nitrous acid, prepared in situ from inorg. nitrite and HCl to give 4-(1H-1,2,4-triazol-1-yl)benzonitrile (3) free of its 4H-1,2,4-triazol-4-yl isomer; reaction of 3 4-fluorobenzonitrile affords 1 with purity ≥99.5% after recrystn. from Et acetate. In an example, 4-bromomethylbenzonitrile (1.53 mol) was heated with 4-amino-4H-1,2,4-triazole (1.683 mol) in 3 L of isopropanol for 5 h at 80-85°; after cooling the reaction mixture to 0-5° the product was filtered and washed with isopropanol and hexane, yielding 310 g (72.2%) of 2; aqueous solution

of 0.982 mol of 2 was then deaminated by 1.963 mol of aqueous HCl and 1.080 mol of NaNO2 at 0-5° for 6 h followed by reaction at 30-35° for 2-3 h; unreacted HNO2 was decomposed with urea, impurities were extracted with dichloromethane, after addition of 25% aqueous ammonia until pH is adjusted to 8.0-8.5 the product 3 was extracted with dichloromethane, concentrated and filtered after addition of isopropanol-hexane (20:80) to give 150 g (82.9%) of 3, free of its 4-triazolyl isomer. The target compound 1 was then prepared by deprotonation of 3 with KOtBu in DMF at -10° to -5° and reaction with 4-fluorobenzonitrile; after neutralization and evaporation of the solvent the crude product was extracted by Et acetate from its aqueous solution and filtered after addition of isopropanol; purification of 1 was achieved by recrystn. from Et acetate to give 58% yield of 1 of 99.90% HPLC purity.

RX(2) OF 6 H + I ===> J...



H I J

YIELD 72%

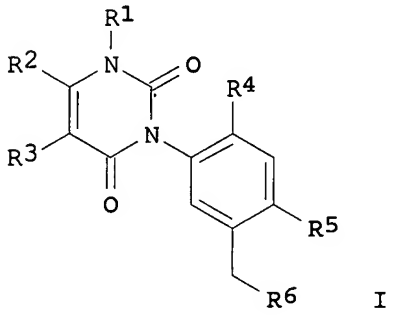
RX(2) RCT H 17201-43-3, I 584-13-4
PRO J **748812-17-1**
SOL 67-63-0 Me2CHOH
CON SUBSTAGE(1) 5 hours, 80 - 85 deg C
SUBSTAGE(2) 85 deg C -> room temperature
SUBSTAGE(3) room temperature -> 5 deg C
SUBSTAGE(4) 2 hours

L50 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN
AN 136:340693 CASREACT
TI Preparation of [(oxotriazolomethyl)phenyl]uracils and analogs as herbicides
IN Andree, Roland; Schwarz, Hans-Georg; Schneider, Udo; Wischnat, Ralf; Drewes, Mark Wilhelm; Dahmen, Peter; Feucht, Dieter; Pontzen, Rolf

PA Bayer Aktiengesellschaft, Germany
SO PCT Int. Appl., 90 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002034725	A1	20020502	WO 2001-EP11589	20011008
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10051981	A1	20020502	DE 2000-10051981	20001020
IN 2001MU00971	A	20050304	IN 2001-MU971	20011005
CA 2425884	A1	20020502	CA 2001-2425884	20011008
AU 200223604	A	20020506	AU 2002-23604	20011008
EP 1330443	A1	20030730	EP 2001-988711	20011008
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001014746	A	20040210	BR 2001-14746	20011008
JP 2004531462	T	20041014	JP 2002-537716	20011008
US 6992044	B1	20060131	US 2003-399359	20030818

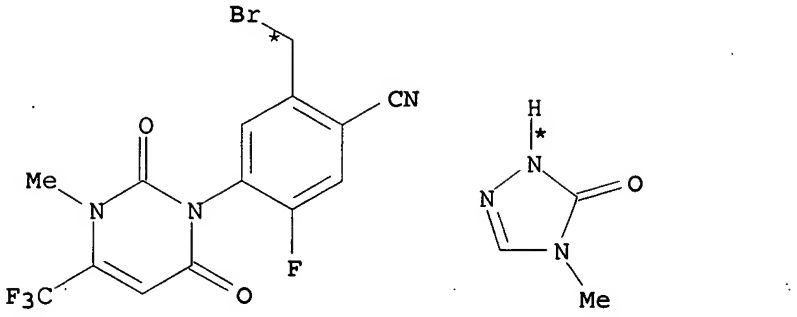
PRAI DE 2000-10051981 20001020
WO 2001-EP11589 20011008
OS MARPAT 136:340693
GI



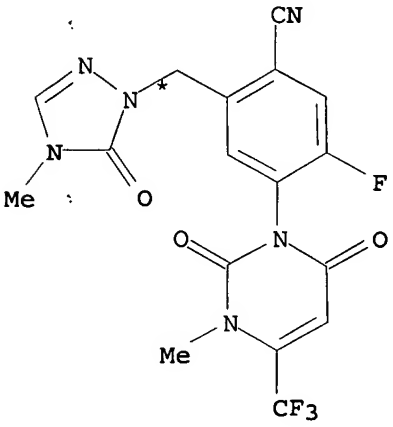
I

AB Title compds. [I; R1 = H, NH2, alk(en)yl, etc.; R2 = cyano, CO2H, CONH2, etc.; R3 = H, halo, (un)substituted alkyl; R4 = H, halo, NO2, cyano, alkoxy; R5 = halo, cyano, CSNH2, alkyl, alkoxy, etc.; R6 = (un)substituted N-attached heterocyclyl] were prepared as herbicides (no data). Thus, RNHCO2Et (R = 4-bromo-2-fluoro-5-methylphenyl) was cyclocondensed with F3CC(NH2):CHCO2Et and the product converted in 2 steps to I (R1 = Me, R2 = CF3, R3 = H, R4 = F, R5 = cyano)(II; R6 = Br) which was aminated by 4-methyl-2,4-dihydro-3H-1,2,4-triazol-3-one to give II (R6 = 4-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-1-yl).

RX(1) OF 28 ...A + B ===> C



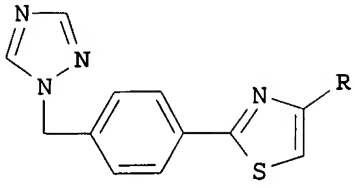
A B (1)



C
YIELD 46%

RX(1) RCT A 418762-20-6, B 4114-43-6
RGT D 584-08-7 K2CO3
PRO C **418762-00-2**
SOL 75-05-8 MeCN
RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN
AN 136:167328 CASREACT
TI Synthesis and antimicrobial activity of 2,4-disubstituted thiazole derivatives containing a 1,2,4-triazole ring system
AU John, Jaya; Bobade, A. S.; Khadse, Barsu G.
CS Haffkine Institute for Training, Research and Testing, Mumbai, 400 012, India
SO Indian Journal of Heterocyclic Chemistry (2001), 10(4), 295-298
CODEN: IJCHEI; ISSN: 0971-1627
PB Prof. R. S. Varma
DT Journal
LA English
GI



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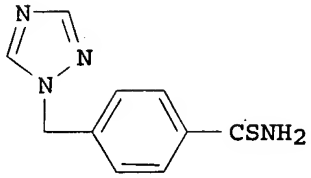
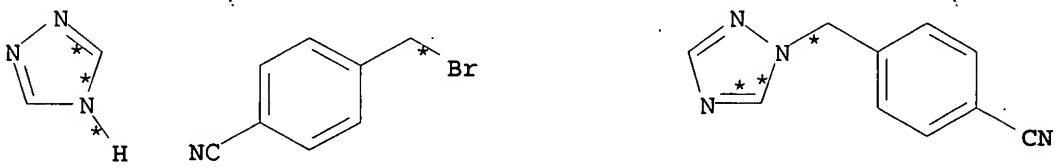


II

AB Title compds. I (R = substituted Ph, 5-chlorothienyl) were prepared by condensation of benzthioamide II with various substituted aryl/heteroaryl α-halo ketones. I were tested for antibacterial activity.

RX(1) OF 39 A + B ===> C...



A B C

(1)

YIELD 57%

RX(1) RCT A 288-88-0, B 17201-43-3

STAGE(1)
SOL 67-66-3 CHCl3, 75-05-8 MeCN

STAGE(2)
RGT D 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO C **112809-25-3**

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> => FILE HCAPL
FILE 'HCAPLUS' ENTERED AT 12:00:05 ON 07 FEB 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

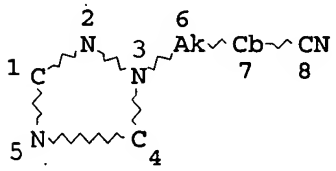
Preps in CA file with condens? or salt? (3A) ? triazol?

FILE COVERS 1907 - 7 Feb 2007 VOL 146 ISS 7
FILE LAST UPDATED: 6 Feb 2007 (20070206/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> D QUE L52
L39 STR

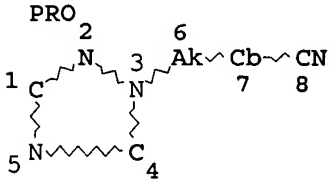


NODE ATTRIBUTES:
CONNECT IS E2 RC AT 6
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 7
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L41 67 SEA FILE=REGISTRY SSS FUL L39
L42 38 SEA FILE=HCAPLUS ABB=ON L41
L43 28 SEA FILE=HCAPLUS ABB=ON L42(L)PREP/RL
L44 1939 SEA FILE=HCAPLUS ABB=ON ?TRIAZOL?(3A)SALT#
L45 1 SEA FILE=HCAPLUS ABB=ON L43 AND L44
L46 8 SEA FILE=HCAPLUS ABB=ON L43 AND CONDENS?
L47 8 SEA FILE=HCAPLUS ABB=ON L45 OR L46
L48 STR

PRO



NODE ATTRIBUTES:
CONNECT IS E2 RC AT 6
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 7
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L50 5 SEA FILE=CASREACT SSS FUL L48 (13 REACTIONS)
L51 5 SEA FILE=HCAPLUS ABB=ON L50

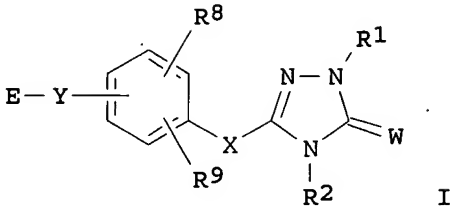
L52 5 SEA FILE=HCAPLUS ABB=ON L47 NOT L51

=> D L52 1-5 BIB ABS IND HITSTR

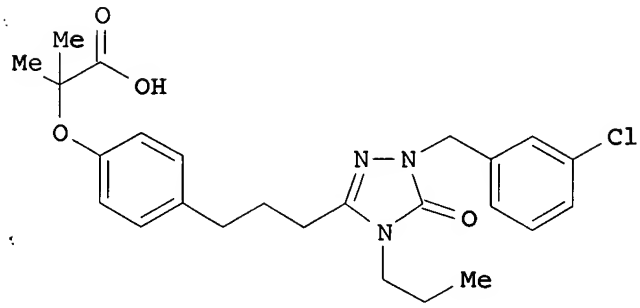
L52 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:368462 HCAPLUS
DN 136:386118
TI Preparation of (phenylalkyl)-1H-[1,2,4]triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions
IN Mantlo, Nathan Bryan; Collado Cano, Ivan; Dominianni, Samuel James; Etgen, Garret Jay, Jr.; Garcia-Paredes, Cristina; Johnston, Richard Duane; Letourneau, Michael Edward; Martinelli, Michael John; Mayhugh, Daniel Ray; Saeed, Ashraf; Thompson, Richard Craig; Wang, Xiadong; Coffey, David Scott; Schmid, Christopher Randall; Vicenzi, Jeffrey Thomas; Xu, Yanping
PA Eli Lilly and Company, USA
SO PCT Int. Appl., 388 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002038553	A2	20020516	WO 2001-US42928	20011109
	WO 2002038553	A3	20030501		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2421154	A1	20020516	CA 2001-2421154	20011109
	AU 200228592	A	20020521	AU 2002-28592	20011109
	EP 1335908	A2	20030820	EP 2001-989704	20011109
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	BR 2001014986	A	20030923	BR 2001-14986	20011109
	HU 200301655	A2	20031229	HU 2003-1655	20011109
	JP 2004513166	T	20040430	JP 2002-541088	20011109
	NZ 524569	A	20060526	NZ 2001-524569	20011109
	IN 2003KN00278	A	20050311	IN 2003-KN278	20030306
	ZA 2003002517	A	20040630	ZA 2003-2517	20030331
	NO 2003002059	A	20030624	NO 2003-2059	20030508
	HR 2003000365	A1	20030831	HR 2003-365	20030508
	US 2004102500	A1	20040527	US 2003-415673	20030911
	AU 2006202811	A1	20060720	AU 2006-202811	20060629
PRAI	US 2000-247317P	P	20001110		
	WO 2001-US42928	W	20011109		

OS MARPAT 136:386118
GI



I



II

AB Title compds. I [wherein R1 = H or (un)substituted alkyl, (hetero)arylalkyl, cycloalkylarylalkyl, CH2COR17R18; R17 = O or NH; R18 = (un)substituted benzyl; W = O or S; R2 = H or (un)substituted (cyclo)alkyl, allyl, (hetero)arylalkyl, sulfonamido, amido, or OR10; R10 = H or alkyl; X = (un)substituted alkylene linker wherein 1 C may be replaced with O, NH, or S; Y = C, O, S, NH, or a single bond; E = H, CR3R4A; A, (un)substituted (CH2)nCO2C19, (aryl)alkyl, allyl, thioalkyl, thioaryl, alkoxyaryl, alkoxyalkyl, aminoaryl, or aminoalkyl; n = 0-3; A = carboxy, alkylnitrile, carboxamide, or (un)substituted sulfonamide, acylsulfonamide, or tetrazole; R3 = H, alkyl, or alkoxy; R4 = H, halo, or (un)substituted (cyclo)alkyl, alkoxy, arylalkyl, or Ph; or CR3R4 = cycloalkyl; R19 = H or (un)substituted arylmethyl or alkyl; R8 = independently H, alkyl, alkenyl, or halo; R9 = independently H, alkenyl, halo, allyl, OR10, or (un)substituted alkyl or (hetero)aryl; R10 = independently H or alkyl] were prepared as peroxisome proliferator activated receptor alpha (PPARα) agonists. For example, **condensation** of 3-chlorobenzaldehyde with 4-(4-hydroxyphenyl)butyrylhydrazide (p-TsOH, i-PrOH), followed by reduction (NaBH3CN, THF, AcOH, i-PrOH), treatment with n-PrNCO (THF), and cyclization (KOH, MeOH), afforded 2-(3-chlorobenzyl)-5-[3-(4-hydroxyphenyl)propyl]-4-propyl-3H-triazolin-3-one. Addition of tert-Bu 2-bromoisobutyrate (K2CO3, DMF) and deesterification (TFA, CH2Cl2) gave II. I bound to PPARα receptors with IC50 values of ≤ 100 nM and demonstrated PPARα cotransfection efficacy in CV-1 cells of ≥ 50%. Significant reduction in RQ in female Ay mice [0.864 ± 0.013 (control) vs. 0.803 ± 0.007 (treated); $p < 0.001$] was observed at doses of 50 mg/kg of I. Addnl., treated animals displayed significantly higher rates of energy expenditure than control animals (17.40 ± 0.49 vs. 13.62 ± 0.26 kcal/kg/h, resp.). Thus, I are useful for the prevention and/or treatment of cardiovascular disease associated with Syndrome X, hyperinsulemia, hypertension, elevated body weight, elevate triglycerides, and elevated LDL.

IC ICM C07D249-12
ICS A61K031-4196; C07D401-06; C07D413-06; C07D409-06; C07D409-12; C07D417-12; C07D405-06; A61K031-4439; A61K031-427; C07C257-22; C07C281-04; C07C281-06

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

ST phenylalkyl triazolone prepn peroxisome proliferator activated receptor alpha agonist; triazolone phenylalkyl prepn Syndrome X treatment; triazolylalkylphenoxy propionate prepn cardiovascular agents

IT Glycerides, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(blood; preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

IT Heart, disease
(cardiac syndrome X, treatment; preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

IT Antihypertensives
Antiobesity agents
Cardiovascular agents
Human
(preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

IT Low-density lipoproteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

IT Peroxisome proliferator-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(α; preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

IT 425669-52-9P 425669-58-5P 425669-59-6P 425669-60-9P 425669-61-0P
425669-62-1P 425669-63-2P 425669-64-3P 425669-65-4P 425669-95-0P
425670-03-7P 425670-33-3P 425670-65-1P 425672-17-9P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(cardiovascular agent; preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

IT 425669-53-0P 425669-54-1P 425669-55-2P 425669-56-3P 425669-57-4P
425669-67-6P 425669-68-7P 425669-69-8P 425669-70-1P 425669-71-2P
425669-72-3P 425669-73-4P 425669-74-5P 425669-75-6P 425669-76-7P
425669-77-8P 425669-78-9P 425669-79-0P 425669-80-3P 425669-81-4P
425669-82-5P 425669-83-6P 425669-84-7P 425669-85-8P 425669-86-9P
425669-87-0P 425669-88-1P 425669-89-2P 425669-90-5P 425669-91-6P
425669-92-7P 425669-93-8P 425669-94-9P 425669-96-1P 425669-97-2P
425669-98-3P 425669-99-4P 425670-00-4P 425670-01-5P 425670-02-6P
425670-04-8P **425670-05-9P** **425670-06-0P** 425670-07-1P
425670-08-2P 425670-09-3P 425670-10-6P 425670-11-7P 425670-12-8P
425670-13-9P 425670-14-0P 425670-15-1P 425670-16-2P 425670-17-3P
425670-18-4P 425670-19-5P 425670-20-8P 425670-21-9P 425670-22-0P
425670-23-1P 425670-24-2P 425670-25-3P 425670-26-4P 425670-28-6P
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425670-46-8P 425670-47-9P **425670-48-0P** 425670-49-1P
425670-50-4P 425670-51-5P 425670-53-7P 425670-56-0P
425670-57-1P 425670-58-2P 425670-59-3P 425670-60-6P 425670-61-7P
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425670-78-6P 425670-80-0P 425670-83-3P **425670-85-5P**
425670-87-7P 425670-89-9P **425670-92-4P** 425670-94-6P
425670-96-8P 425670-98-0P 425670-99-1P 425671-00-7P 425671-01-8P
425671-02-9P 425671-03-0P 425671-04-1P 425671-05-2P
425671-06-3P 425671-07-4P 425671-08-5P 425671-11-0P
425671-12-1P 425671-13-2P 425671-14-3P 425671-15-4P 425671-16-5P
425671-17-6P 425671-18-7P 425671-19-8P **425671-20-1P**
425671-21-2P 425671-22-3P 425671-23-4P 425671-24-5P 425671-25-6P
425671-26-7P 425671-27-8P 425671-28-9P 425671-29-0P 425671-30-3P
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425671-41-6P 425671-42-7P 425671-43-8P 425671-44-9P 425671-45-0P
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425671-81-4P 425671-82-5P 425671-83-6P 425671-84-7P 425671-85-8P
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425671-96-1P 425671-97-2P 425671-98-3P 425671-99-4P 425672-00-0P
425672-01-1P 425672-02-2P, 2-[4-[3-[1-(3-Methoxybenzyl)-5-oxo-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methylpropionic acid
425672-03-3P 425672-04-4P 425672-05-5P 425672-06-6P 425672-07-7P, 2-Methyl-2-[4-[2-[5-oxo-4-propyl-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]ethyl]phenoxy]propionic acid 425672-08-8P, [4-[2-[5-Oxo-4-propyl-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]ethyl]phenoxy]acetic acid 425672-09-9P 425672-10-2P
425672-11-3P, [4-[2-[4-[2-(2-Fluorophenyl)ethyl]-5-oxo-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]ethyl]phenoxy]acetic acid 425672-12-4P, 2-[4-[2-[4-[2-(2-Fluorophenyl)ethyl]-5-oxo-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]ethyl]phenoxy]-2-methylpropionic acid 425672-13-5P, [4-[3-[4-[2-(2-Fluorophenyl)ethyl]-5-oxo-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]phenoxy]acetic acid 425672-14-6P, 2-[4-[3-[4-[2-(2-Fluorophenyl)ethyl]-5-oxo-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methylpropionic acid
425672-15-7P 425672-16-8P 425672-18-0P 425672-19-1P, [2-Iodo-4-[2-[5-oxo-4-propyl-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]ethyl]phenoxy]acetic acid 425672-20-4P, [4-[2-[4-[2-(2-Fluorophenyl)ethyl]-5-oxo-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]ethyl]-2-methylphenoxy]acetic acid
425672-21-5P, 2-[4-[2-[4-[2-(2-Fluorophenyl)ethyl]-5-oxo-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]ethyl]-2-methylphenoxy]-2-methylpropionic acid 425672-22-6P, [4-[3-[4-[2-(2-Fluorophenyl)ethyl]-5-oxo-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]-2-methylphenoxy]acetic acid 425672-23-7P, 2-[4-[3-[4-[2-(2-Fluorophenyl)ethyl]-5-oxo-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]-2-methylphenoxy]-2-methylpropionic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(cardiovascular agent; preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

IT 425672-24-8P 425672-25-9P 425672-26-0P 425672-27-1P 425672-29-3P
425672-30-6P 425672-31-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cardiovascular agent; preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

IT 9004-10-8, Insulin, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hyperinsulinemia, treatment; preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

IT 13923-56-3P 15823-04-8P 20637-08-5P, Methyl 4-(4-methoxyphenyl)butyrate 22320-10-1P, Methyl 4-(4-hydroxyphenyl)butyrate 24469-50-9P 31600-43-8P 34674-93-6P, 4-(4-Hydroxyphenyl)butyric Acid 50704-52-4P 51336-47-1P 53370-84-6P 57676-49-0P 92547-53-0P 105238-87-7P, 3-(4-Methoxyphenyl)-N-propylpropionamide 106728-61-4P 112961-39-4P 121670-33-5P 123566-47-2P 162739-90-4P 194163-50-3P 237064-46-9P 348162-63-0P 402617-08-7P 402723-13-1P 425669-66-5P 425672-32-8P 425672-33-9P 425672-34-0P 425672-35-1P 425672-36-2P 425672-37-3P 425672-38-4P 425672-39-5P 425672-40-8P 425672-41-9P 425672-42-0P 425672-43-1P 425672-44-2P 425672-45-3P 425672-46-4P 425672-47-5P 425672-48-6P 425672-49-7P 425672-50-0P 425672-51-1P 425672-52-2P 425672-53-3P 425672-54-4P 425672-55-5P 425672-56-6P 425672-57-7P 425672-58-8P 425672-59-9P 425672-60-2P 425672-61-3P 425672-62-4P 425672-63-5P 425672-64-6P 425672-65-7P 425672-66-8P 425672-67-9P 425672-68-0P 425672-69-1P 425672-70-4P 425672-71-5P 425672-72-6P 425672-73-7P 425672-74-8P 425672-75-9P 425672-76-0P 425672-77-1P 425672-78-2P 425672-79-3P 425672-80-6P 425672-81-7P 425672-82-8P 425672-83-9P 425672-84-0P 425672-85-1P 425672-86-2P 425672-87-3P 425672-88-4P 425672-89-5P 425672-90-8P 425672-91-9P 425672-92-0P 425672-93-1P 425672-94-2P 425672-95-3P 425672-96-4P 425672-97-5P 425672-98-6P 425672-99-7P 425673-00-3P 425673-01-4P 425673-02-5P 425673-03-6P 425673-04-7P 425673-05-8P 425673-06-9P 425673-07-0P 425673-08-1P 425673-09-2P 425673-10-5P 425673-11-6P 425673-12-7P 425673-13-8P 425673-14-9P **425673-15-0P** **425673-16-1P** 425673-17-2P 425673-18-3P 425673-19-4P 425673-20-7P 425673-21-8P 425673-22-9P 425673-23-0P 425673-24-1P 425673-25-2P 425673-26-3P 425673-27-4P 425673-28-5P 425673-29-6P 425673-30-9P 425673-31-0P 425673-32-1P 425673-33-2P 425673-34-3P 425673-35-4P 425673-36-5P 425673-37-6P 425673-38-7P 425673-39-8P 425673-40-1P 425673-41-2P 425673-42-3P 425673-43-4P 425673-44-5P 425673-45-6P 425673-46-7P 425673-47-8P 425673-48-9P 425673-49-0P 425673-50-3P 425673-51-4P 425673-52-5P 425673-53-6P 425673-54-7P 425673-55-8P 425673-56-9P 425673-57-0P 425673-58-1P 425673-59-2P 425673-60-5P **425673-61-6P** 425673-62-7P **425673-63-8P** 425673-64-9P 425673-65-0P 425673-66-1P 425673-67-2P 425673-68-3P 425673-69-4P 425673-70-7P 425673-71-8P 425673-72-9P 425673-73-0P 425673-74-1P 425673-75-2P 425673-76-3P 425673-77-4P 425673-78-5P 425673-79-6P 425673-80-9P 425673-81-0P 425673-82-1P 425673-83-2P 425673-84-3P 425673-85-4P 425673-86-5P **425673-87-6P** 425673-88-7P 425673-89-8P **425673-90-1P** 425673-91-2P 425673-92-3P 425673-93-4P 425673-94-5P 425673-95-6P 425673-96-7P 425673-97-8P 425673-98-9P 425673-99-0P 425674-00-6P **425674-01-7P** 425674-02-8P 425674-03-9P 425674-04-0P 425674-05-1P 425674-06-2P 425674-07-3P 425674-08-4P 425674-09-5P 425674-10-8P 425674-11-9P 425674-12-0P 425674-13-1P 425674-14-2P 425674-15-3P 425674-16-4P 425674-17-5P 425674-18-6P 425674-19-7P 425674-20-0P 425674-21-1P 425674-22-2P 425674-23-3P 425674-24-4P 425674-25-5P 425674-26-6P 425674-27-7P 425674-28-8P 425674-29-9P 425674-30-2P 425674-31-3P 425674-32-4P 425674-33-5P 425674-34-6P

425674-35-7P 425674-36-8P 425674-37-9P 425674-38-0P 425674-39-1P
425674-40-4P 425674-41-5P 425674-42-6P 425674-43-7P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

IT 425674-44-8P 425674-45-9P 425674-46-0P 425674-47-1P 425674-48-2P
425674-49-3P 425674-50-6P 425674-51-7P 425674-52-8P 425674-53-9P
425674-54-0P 425674-55-1P 425674-56-2P 425674-57-3P 425674-58-4P
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425674-64-2P 425674-65-3P 425674-66-4P 425674-67-5P 425674-68-6P
425674-69-7P 425674-70-0P 425674-71-1P 425674-72-2P 425674-73-3P
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425674-89-1P 425674-90-4P 425674-91-5P 425674-92-6P 425674-93-7P
425674-94-8P 425674-95-9P 425674-96-0P 425674-97-1P 425674-98-2P
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425675-04-3P 425675-05-4P 425675-06-5P 425675-07-6P 425675-08-7P
425675-09-8P 425675-10-1P 425675-11-2P 425675-12-3P 425675-13-4P
425675-14-5P 425675-15-6P 425675-16-7P 425675-17-8P,
2-[4-[3-[1-(4-tert-Butylbenzyl)-4-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-3-(4-fluorophenyl)-2-methylpropionic acid ethyl ester 425675-18-9P 425675-19-0P 425675-20-3P 425675-21-4P,
2-Methyl-2-[4-[3-[4-methyl-5-oxo-1-(3-trifluoromethylbenzyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-3-phenylpropionic acid ethyl ester
425675-22-5P 425675-23-6P 425675-24-7P, 2-[4-[3-[4-Methyl-5-oxo-1-(3-phenoxybenzyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]phenoxy]propionic acid ethyl ester 425675-25-8P, 2-Methyl-2-[4-[3-[4-methyl-5-oxo-1-(3-phenoxybenzyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-3-phenylpropionic acid ethyl ester 425675-26-9P 425675-27-0P
425675-29-2P 425675-30-5P 425675-31-6P, 2-[4-[3-[1-(3-Methoxybenzyl)-5-oxo-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methylpropionic acid ethyl ester 425675-32-7P 425675-33-8P 425675-34-9P
425675-35-0P 425675-36-1P 425675-37-2P 425675-39-4P 425675-40-7P
425675-41-8P, 2-Methyl-2-[4-[3-[1-(4-methylbenzyl)-5-oxo-4-propyl-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]phenoxy]propionic acid ethyl ester
425675-42-9P, 4-[4-(1-Ethoxycarbonyl-1-methylethoxy)phenyl]butyric acid
425675-43-0P 425675-45-2P 425675-46-3P 425675-48-5P 425675-50-9P
425675-51-0P 425675-52-1P, 2-[4-[3-[1-(3,5-Difluorobenzyl)-5-oxo-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methylpropionic acid ethyl ester 425675-53-2P 425675-54-3P 425675-56-5P 425675-57-6P
425675-58-7P 425675-59-8P 425675-60-1P 425675-62-3P 425675-63-4P
425675-64-5P, 2-[4-[3-(1-Phenylmethyl-5-oxo-4-propyl-4,5-dihydro-1H-1,2,4-triazol-3-yl)propyl]phenoxy]-2-methylpropionic acid ethyl ester
425675-65-6P 425675-66-7P 425675-67-8P 425675-68-9P 425675-70-3P
425675-71-4P 425675-72-5P, 2-[4-[3-[4-Ethyl-1-(naphthalen-2-yl)methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methylpropionic acid ethyl ester 425675-73-6P 425675-74-7P 425675-75-8P
425675-76-9P 425675-78-1P 425675-79-2P 425675-80-5P 425675-81-6P
425675-82-7P 425675-84-9P 425675-85-0P 425675-86-1P,
2-[4-[3-[1-(4-tert-Butylphenylmethyl)-4-methyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methylpropionic acid ethyl ester
425675-87-2P, 3-(4-Methoxyphenyl)-N-propylpropionimidic acid methyl ester
425675-88-3P 425675-89-4P 425675-90-7P 425675-91-8P,
2-Methyl-2-[4-[2-[5-oxo-4-propyl-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]ethyl]phenoxy]propionic acid ethyl ester
425675-92-9P, [2-Iodo-4-[2-[5-oxo-4-propyl-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]ethyl]phenoxy]acetic acid ethyl ester

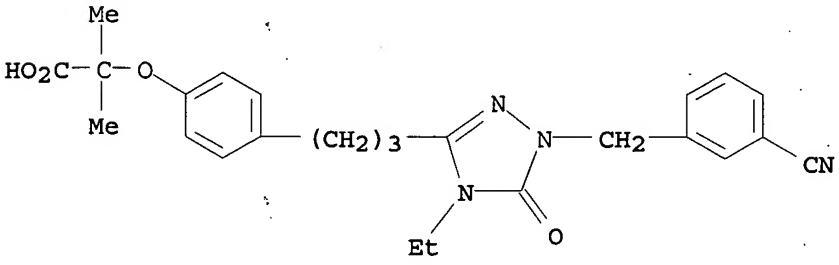
425675-94-1P 425675-95-2P 425675-96-3P 425675-97-4P 425675-98-5P
425675-99-6P 425676-00-2P 425676-01-3P 425676-02-4P 425676-03-5P
425676-04-6P 425676-05-7P 425676-06-8P 425676-07-9P 425676-08-0P
425676-09-1P 425676-10-4P 425676-11-5P 425676-12-6P 425676-13-7P
425676-15-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

IT 66-99-9, 2-Naphthaldehyde 96-32-2, Methyl bromoacetate 98-10-2, Benzenesulfonamide 102-46-5, 3,4-Dimethylbenzyl chloride 102-48-7, 3,4-Dimethylbenzylamine 103-63-9, Phenethyl bromide 104-81-4, 4-Methylbenzyl bromide 104-82-5, α-Chloro-p-xylene 104-84-7, 4-Methylbenzylamine 104-87-0, p-Methyl benzaldehyde 105-13-5, 4-Methoxybenzyl alcohol 105-36-2, Ethyl bromoacetate 109-90-0, Ethyl isocyanate 110-78-1, Propyl isocyanate 111-36-4, Butyl isocyanate 368-90-1, 4-Trifluoromethylphenylhydrazine 402-23-3, 3-Trifluoromethylbenzyl bromide 452-35-7, 6-Ethoxy-2-benzothiazolesulfonamide 459-46-1, 4-Fluorobenzyl bromide 513-38-2, 1-Iodo-2-methylpropane 535-11-5, Ethyl 2-bromopropionate 587-04-2, 3-Chlorobenzaldehyde 591-31-1, m-Anisaldehyde 592-55-2, 2-Bromoethyl ethyl ether 600-00-0, Ethyl 2-bromoisobutyrate 620-24-6, 3-Hydroxybenzyl alcohol 627-18-9, 1-Bromo-3-hydroxypropane 637-59-2, 3-Phenylpropyl bromide 765-30-0, Cyclopropylamine 766-80-3, m-Chlorobenzyl bromide 816-40-0, 1-Bromobutan-2-one 870-46-2, tert-Butyl carbazate 927-68-4, 2-Bromoethyl acetate 939-26-4, 2-Bromomethylnaphthalene 939-97-9, 4-tert-Butylbenzaldehyde 1129-26-6, 4-Methoxybenzenesulfonamide 1576-47-2, Naphthalene-2-sulfonamide 1761-61-1, 5-Bromosalicylaldehyde 1929-29-9, 3-(4-Methoxyphenyl)propionic acid 2525-62-4, Hexyl isocyanate 2969-81-5, Ethyl 4-bromobutyrate 3173-56-6, Benzyl isocyanate 3395-91-3 3840-30-0, 3,4,5-Trimethoxybenzyl chloride 3954-13-0, Pentyl isocyanate 4377-33-7, 2-Chloromethylpyridine 4521-28-2, 4-(4-Methoxyphenyl)butyric acid 4563-33-1, α-Toluenesulfonamide 4897-84-1, Methyl 4-bromobutyrate 5071-96-5, 3-Methoxybenzylamine 5406-18-8, 3-(4-Methoxyphenyl)-1-propanol 5437-45-6, Benzyl bromoacetate 5469-26-1, 1-Bromo-3,3-dimethylbutan-2-one 5973-71-7, 3,4-Dimethylbenzaldehyde 6065-66-3, 2-Bromoethylbutyrate 6287-38-3, 3,4-Dichlorobenzaldehyde 6482-24-2, 2-Bromoethyl methyl ether 7051-34-5, Bromomethylcyclopropane 10385-30-5, 4-Benzyloxybutyric acid 10445-91-7, 4-Chloromethylpyridine 10516-71-9, 3-(3-Methoxyphenyl)propionic acid 16889-72-8, tert-Butyl isobutyrate 17260-71-8, 3-Chlorobenzenesulfonamide 18880-00-7, 4-(tert-Butyl)benzyl bromide 23786-14-3, Methyl 4-methoxyphenylacetate 23877-12-5, tert-Butyl 2-bromoisobutyrate 27129-86-8, 3,5-Dimethylbenzyl bromide 27913-58-2, 4-(p-Iodophenyl)butyric acid 30379-55-6, Benzyloxyacetic acid 31469-15-5, 1-Methoxy-1-trimethylsiloxy-2-methyl-1-propene 32085-88-4, 3,5-Difluorobenzaldehyde 36978-34-4, 4-Bromobutyl benzoate 52244-70-9, 4-(4-Methoxyphenyl)-1-butanol 53595-65-6, 5-Bromothiophene-2-sulfonamide 53874-66-1, 3-Phenoxybenzyl chloride 57816-01-0 58336-71-3, Ethyl 2-[4-(bromomethyl)phenoxy]-2-methylpropionate 93489-13-5, 2,4-Dimethoxybenzyl isocyanate 93489-19-1, 2,4,6-Trimethoxybenzyl isocyanate 94416-66-7, 3,4-Dimethylbenzyl bromide 152270-53-6, 2-(4-Hydroxyphenyl)-2-methylpropanoic acid ethyl ester 166960-23-2 247923-30-4, tert-Butyl 2-(4-bromophenylsulfanyl)-2-methylpropionate 425675-93-0, [4-[2-[5-Oxo-4-propyl-1-(4-trifluoromethylphenyl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]ethyl]phenoxy]acetic acid ethyl ester 425676-19-3 425676-20-6

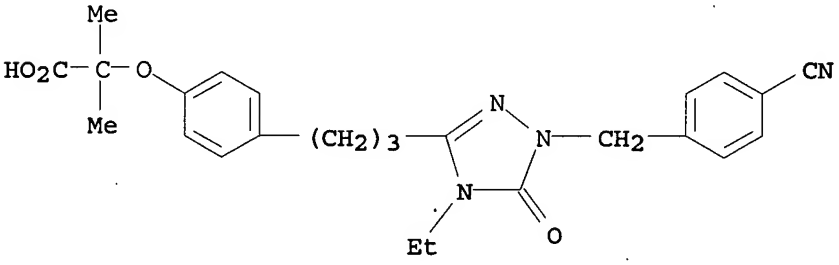
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

IT **425670-05-9P 425670-06-0P 425670-48-0P**
425670-50-4P 425670-85-5P 425670-92-4P
425671-06-3P 425671-17-6P 425671-20-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(cardiovascular agent; preparation of (phenylalkyl)triazolones as PPARα agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

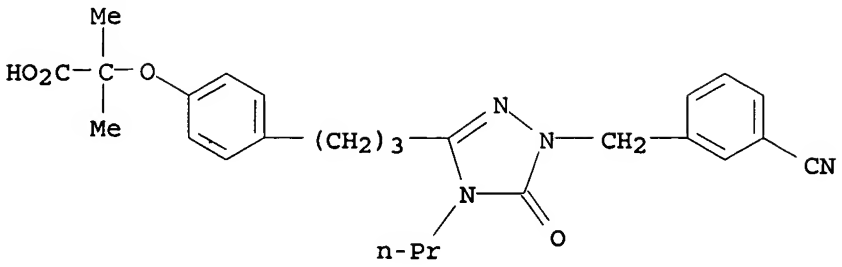
RN 425670-05-9 HCAPLUS
CN Propanoic acid, 2-[4-[3-[1-[(3-cyanophenyl)methyl]-4-ethyl-4,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)



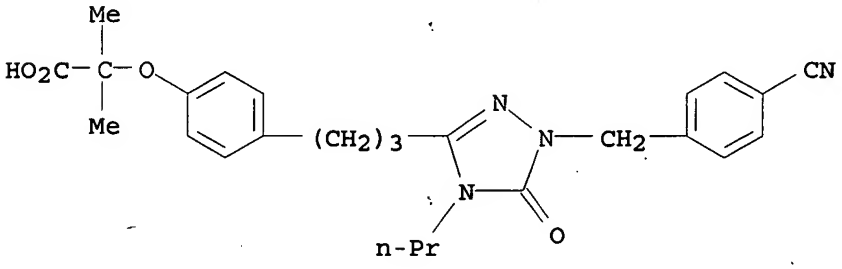
RN 425670-06-0 HCAPLUS
CN Propanoic acid, 2-[4-[3-[1-[(4-cyanophenyl)methyl]-4-ethyl-4,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)



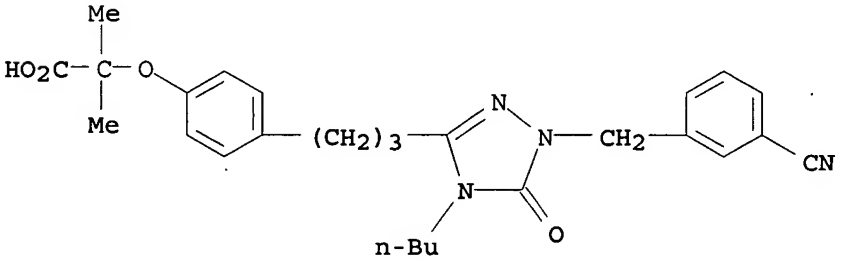
RN 425670-48-0 HCAPLUS
CN Propanoic acid, 2-[4-[3-[1-[(3-cyanophenyl)methyl]-4,5-dihydro-5-oxo-4-propyl-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)



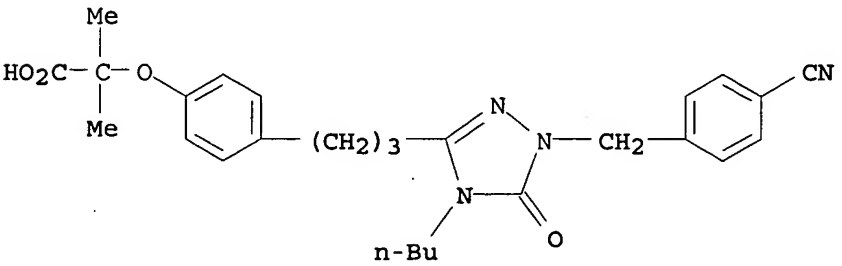
RN 425670-50-4 HCAPLUS
CN Propanoic acid, 2-[4-[3-[1-[(4-cyanophenyl)methyl]-4,5-dihydro-5-oxo-4-propyl-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)



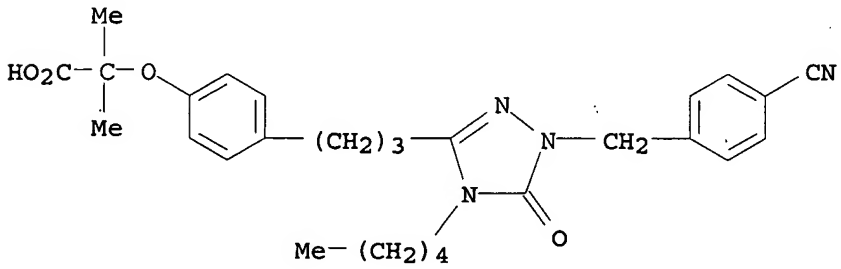
RN 425670-85-5 HCAPLUS
CN Propanoic acid, 2-[4-[3-[4-butyl-1-[(3-cyanophenyl)methyl]-4,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)



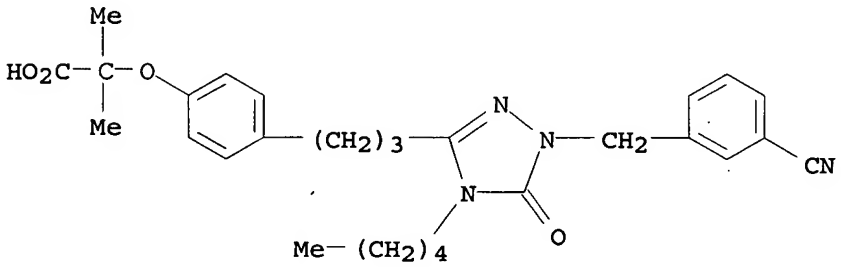
RN 425670-92-4 HCAPLUS
CN Propanoic acid, 2-[4-[3-[4-butyl-1-[(4-cyanophenyl)methyl]-4,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)



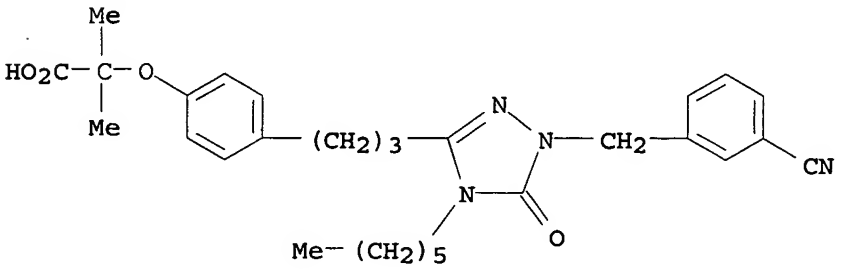
RN 425671-06-3 HCAPLUS
CN Propanoic acid, 2-[4-[3-[1-[(4-cyanophenyl)methyl]-4,5-dihydro-5-oxo-4-pentyl-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)



RN 425671-17-6 HCAPLUS
CN Propanoic acid, 2-[4-[3-[1-[(3-cyanophenyl)methyl]-4,5-dihydro-5-oxo-4-pentyl-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)



RN 425671-20-1 HCAPLUS
CN Propanoic acid, 2-[4-[3-[1-[(3-cyanophenyl)methyl]-4-hexyl-4,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

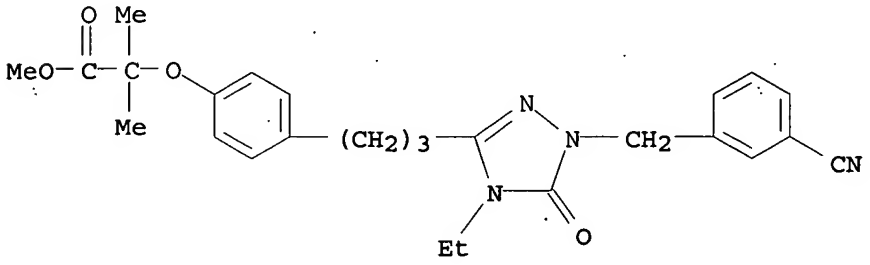


IT **425673-15-0P 425673-16-1P 425673-61-6P**
425673-63-8P 425673-87-6P 425673-90-1P
425674-01-7P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; preparation of (phenylalkyl)triazolones as PPARα

agonists for treatment of cardiovascular disease associated with Syndrome X and related conditions)

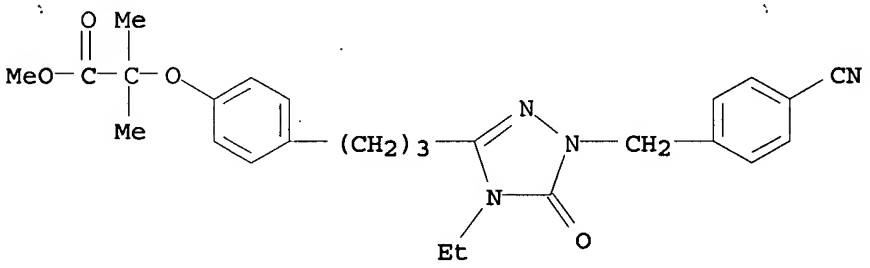
RN 425673-15-0 HCAPLUS

CN Propanoic acid, 2-[4-[3-[1-[(3-cyanophenyl)methyl]-4-ethyl-4,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)



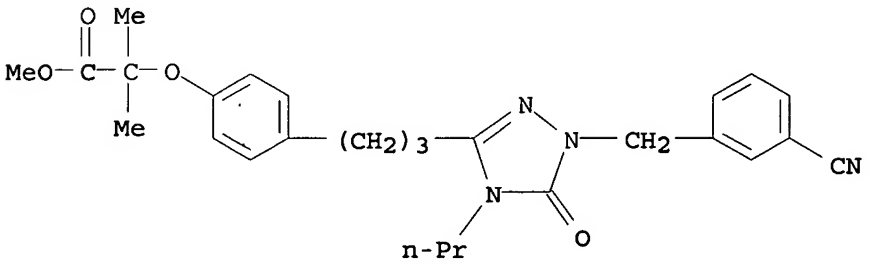
RN 425673-16-1 HCAPLUS

CN Propanoic acid, 2-[4-[3-[1-[(4-cyanophenyl)methyl]-4-ethyl-4,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)



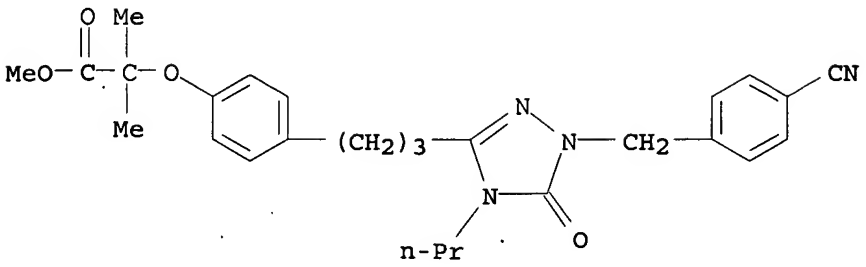
RN 425673-61-6 HCAPLUS

CN Propanoic acid, 2-[4-[3-[1-[(3-cyanophenyl)methyl]-4,5-dihydro-5-oxo-4-propyl-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)

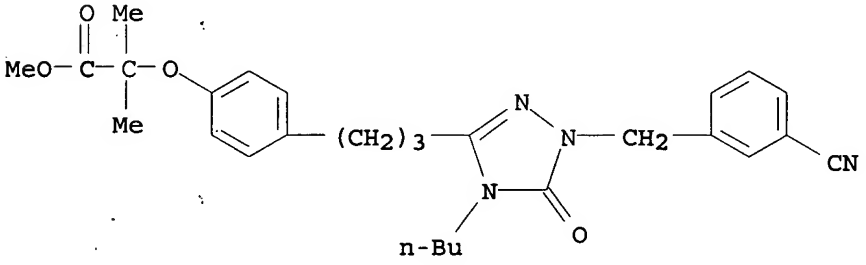


RN 425673-63-8 HCAPLUS

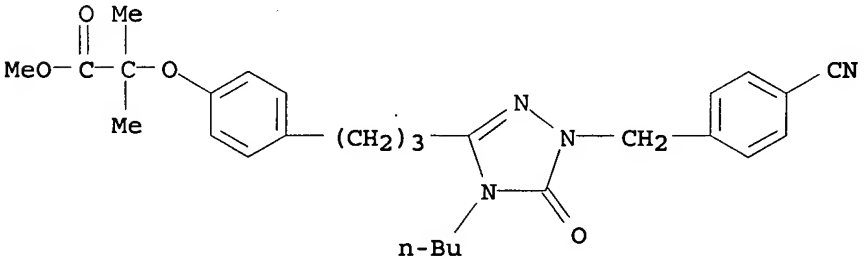
CN Propanoic acid, 2-[4-[3-[1-[(4-cyanophenyl)methyl]-4,5-dihydro-5-oxo-4-propyl-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)



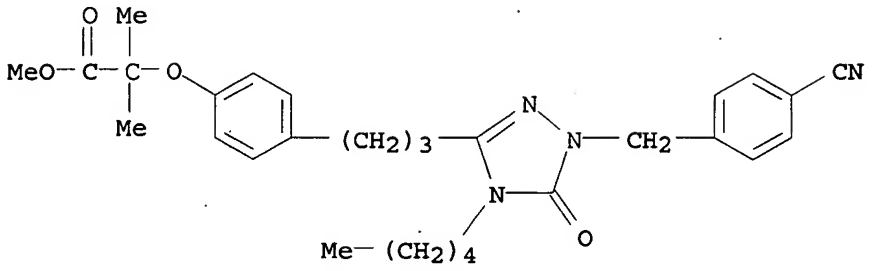
RN 425673-87-6 HCAPLUS
CN Propanoic acid, 2-[4-[3-[4-butyl-1-[(3-cyanophenyl)methyl]-4,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 425673-90-1 HCAPLUS
CN Propanoic acid, 2-[4-[3-[4-butyl-1-[(4-cyanophenyl)methyl]-4,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 425674-01-7 HCAPLUS
CN Propanoic acid, 2-[4-[3-[1-[(4-cyanophenyl)methyl]-4,5-dihydro-5-oxo-4-pentyl-1H-1,2,4-triazol-3-yl]propyl]phenoxy]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)



L52 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:249082 HCAPLUS
DN 130:282071
TI Preparation of prenyl-protein transferase inhibitors
IN Desolms, S. Jane; Hutchinson, John H.; Shaw, Anthony W.; Graham, Samuel L.; Ciccarone, Terrence M.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 202 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9917777	A1	19990415	WO 1998-US21063	19981007
	W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6297239	B1	20011002	US 1998-167180	19981006
	CA 2306746	A1	19990415	CA 1998-2306746	19981007
	AU 9897883	A	19990427	AU 1998-97883	19981007
	AU 741945	B2	20011213		
	EP 1021188	A1	20000726	EP 1998-952110	19981007
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	JP 2001518508	T	20011016	JP 2000-514648	19981007
PRAI	US 1997-62660P	P	19971008		
	WO 1998-US21063	W	19981007		

OS MARPAT 130:282071
AB R4A4Z4ZA1Z1A2Z2XZ3A3Z5R5 [I; A1-A3 = bond, O, CO, CH:CH, (alkyl)imino, etc.; A4 = bond, CO, C(:CH2), etc.; R4 = H, (un)substituted heterocyclyl, -aryl; R5 = cycloalkyl, heterocyclyl, aryl, etc.; X = bond, (un)substituted cycloalkylene, -arylene, -heterocyclylene; Z = (un)substituted C6H4; Z1-Z4 = bond or (un)substituted alkylene; A1Z1A2Z2XZ3A3Z5 ≠ bond] were prepared Thus, Ph 4-amino-2-hydroxybenzoate was converted in 5 steps to R4CH2ZOCH2C6H4(Ph)-4 (II; Z = 4-cyano-1,2-phenylene)(III; R4 = OSO2Me) which was **condensed** with imidazole to give III (R4 = 1-imidazolyl). Data for biol. activity of I were given.
IC ICM A61K031-535
ICS A61K031-44; A61K031-415; C07D413-00; C07D401-00; C07D417-00; C07D419-00; C07D233-66

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
ST prenyl protein transferase inhibitor prepn
IT Antitumor agents
Prenylation
(preparation of prenyl-protein transferase inhibitors)
IT 222975-78-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Preparation of prenyl-protein transferase inhibitors)
IT 222978-32-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of prenyl-protein transferase inhibitors)
IT 222975-79-3P 222975-80-6P 222975-81-7P 222975-82-8P 222975-83-9P
222975-85-1P 222975-86-2P 222975-87-3P 222975-88-4P 222975-89-5P
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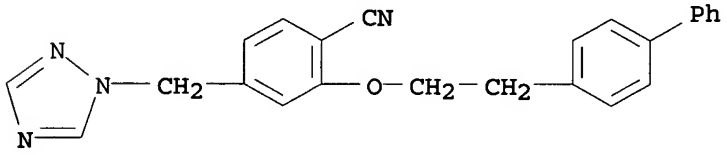
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of prenyl-protein transferase inhibitors)
IT 95-57-8, 2-Chlorophenol 108-42-9, 3-Chloroaniline 108-43-0, 3-Chlorophenol 133-11-9, Phenyl 4-amino-2-hydroxybenzoate 135-19-3,

2-Naphthol, reactions 142-08-5, 2(1H)-Pyridinone 288-32-4, Imidazole, reactions 452-74-4, 4-Bromo-3-fluorotoluene 529-28-2, 2-Iodoanisole 873-77-8, 4-Chlorophenylmagnesium bromide 1122-41-4, 2,4-Dichlorothiophenol 1875-88-3, 2-(4-Chlorophenyl)ethanol 2185-03-7, L-Homoserine lactone hydrochloride 2374-03-0, 4-Amino-3-hydroxybenzoic acid 3510-66-5, 2-Bromo-5-methylpyridine 4214-79-3, 5-Chloro-2-pyridinol 5150-42-5, 2,3-Dimethoxyphenol 5292-21-7, Cyclohexaneacetic acid 14704-31-5 18113-03-6, 2-Chloro-4-methoxyphenol 32316-92-0, 2-Naphthylboronic acid 32673-41-9, Imidazole-4-methanol hydrochloride 51721-15-4, Nγ-Pivaloyloxymethyl-Nα-phthaloylhistamine 72762-00-6, 2-Pyridinol 73373-17-8 96797-15-8, 4-Iodo-1-trityl-1H-imidazole 178685-10-4, 4-(2-Iodoethyl)-1,1'-biphenyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of prenyl-protein transferase inhibitors)

IT 6520-87-2P, Methyl 4-cyano-3-hydroxybenzoate 33769-07-2P 40856-59-5P 63435-16-5P, Methyl 4-amino-3-hydroxybenzoate 101048-76-4P, 2-Fluoro-4-formylbenzonitrile 133059-43-5P, 4-Bromo-3-fluorobenzaldehyde 153556-42-4P, 4-Bromo-3-fluorobenzoic acid 157942-12-6P, Methyl 3-hydroxy-4-iodobenzoate 183500-34-7P 183500-42-7P 183500-44-9P 210037-29-9P 210037-30-2P 210037-55-1P, 2-Hydroxy-4-hydroxymethylbenzonitrile 210037-56-2P, 4-Bromomethyl-2-hydroxybenzonitrile 210037-57-3P 222977-90-4P 222977-91-5P 222977-92-6P 222977-93-7P 222977-94-8P, Phenyl 4-cyano-2-hydroxybenzoate 222977-95-9P 222977-96-0P 222977-97-1P 222977-98-2P 222977-99-3P 222978-00-9P 222978-01-0P, 4-Bromo-3-fluorobenzenemethanol 222978-02-1P, 2-Fluoro-4-hydroxymethylbenzonitrile 222978-03-2P, 4-Bromomethyl-2-fluorobenzonitrile 222978-04-3P 222978-05-4P 222978-06-5P 222978-07-6P 222978-08-7P 222978-09-8P 222978-10-1P 222978-11-2P 222978-12-3P 222978-13-4P 222978-14-5P 222978-15-6P 222978-16-7P 222978-17-8P 222978-18-9P 222978-19-0P 222978-20-3P 222978-21-4P 222978-22-5P 222978-23-6P 222978-24-7P 222978-25-8P 222978-26-9P 222978-27-0P 222978-28-1P 222978-29-2P 222978-30-5P 222978-31-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of prenyl-protein transferase inhibitors)

IT **222975-96-4P 222977-61-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of prenyl-protein transferase inhibitors)

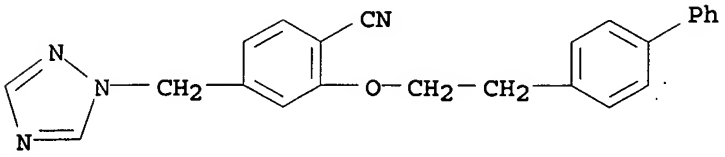
RN 222975-96-4 HCAPLUS
CN Benzonitrile, 2-(2-[1,1'-biphenyl]-4-ylethoxy)-4-(1H-1,2,4-triazol-1-ylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



O HCl

RN 222977-61-9 HCAPLUS
CN Benzonitrile, 2-(2-[1,1'-biphenyl]-4-ylethoxy)-4-(1H-1,2,4-triazol-1-

ylmethyl)- (9CI) (CA INDEX NAME)



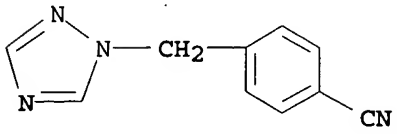
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L52 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 1991:247288 HCAPLUS
DN 114:247288
TI Preparation of cycloalkyleneazoles as aromatase inhibitors
IN Bohlmann, Rolf; Strehlke, Peter; Henderson, David; Schneider, Martin; Nishino, Yukishige
PA Schering A.-G., Germany
SO Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 411735	A1	19910206	EP 1990-250201	19900806
	EP 411735	B1	19950517		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	DE 3926365	A1	19910207	DE 1989-3926365	19890804
	DD 296917	A5	19911219	DD 1990-343215	19900802
	CA 2022682	A1	19910205	CA 1990-2022682	19900803
	CA 2022682	C	19970121		
	AU 9060194	A	19910207	AU 1990-60194	19900803
	AU 634266	B2	19930218		
	ZA 9006150	A	19910529	ZA 1990-6150	19900803
	US 5135937	A	19920804	US 1990-563114	19900803
	IL 95279	A	19950330	IL 1990-95279	19900803
	CN 1049157	A	19910213	CN 1990-106813	19900804
	CN 1024345	B	19940427		
	WO 9101975	A1	19910221	WO 1990-DE611	19900806
	W: FI, HU, JP, NO				
	HU 59911	A2	19920728	HU 1992-324	19900806
	HU 217126	B	19991129		
	JP 05501104	T	19930304	JP 1990-510807	19900806
	JP 3207417	B2	20010910		
	ES 2074530	T3	19950916	ES 1990-250201	19900806
	NO 9200432	A	19920203	NO 1992-432	19920203
	NO 301115	B1	19970915		
	US 5280035	A	19940118	US 1992-889331	19920528
	US 5411982	A	19950502	US 1993-153326	19931116
	NO 9604916	A	19920203	NO 1996-4916	19961119
	FI 9700166	A	19970115	FI 1997-166	19970115
PRAI	DE 1989-3926365	A	19890804		
	US 1990-563114	A3	19900803		
	WO 1990-DE611	W	19900806		
	FI 1992-425	A	19920130		
	NO 1992-432	A	19920203		

US 1992-889331 A3 19920528
OS CASREACT 114:247288; MARPAT 114:247288
GI For diagram(s), see printed CA Issue.
AB Title compds. [I; W = atoms to complete an alkyl-substituted (poly)carbocyclic ring; X = CH:CH, O, S; Y, Z = CH, N], were prepared Thus, imidazole in DMF was treated with NaH and then 4-bromomethylbenzonitrile to give 4-(1-imidazolylmethyl)benzonitrile. The latter in THF at -50° was treated with LiN(CHMe2)2 in THF and then with cyclohexanone at -60° to give the hydroxycyclohexyl derivative, which was refluxed with SOCl2 to give title compound II. II at 2 mg/kg/day gave 74% inhibition of androstenedione-induced uterine weight gain in rats.
IC ICM C07D233-58
ICS C07D249-08; C07D249-04; C07D409-06; A61K031-41
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
ST cycloalkyleneazole prepn aromatase inhibitor; imidazole cycloalkylene prepn aromatase inhibitor
IT 7333-51-9, Cyclohexyltriphenylphosphonium bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of, with cyanothiophenecarboxaldehyde)
IT 72835-25-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of, in preparation of cycloalkyleneazole aromatase inhibitor)
IT 9039-48-9, Aromatase
RL: USES (Uses)
(inhibitors, preparation of cycloalkyleneazoles as)
IT 7311-46-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and **condensation** of, with imidazole, in preparation of aromatase inhibitor)
IT 134134-96-6P 134134-97-7P 134134-98-8P 134134-99-9P 134135-00-5P
134135-01-6P 134135-02-7P 134135-03-8P 134135-04-9P 134135-05-0P
134135-06-1P 134135-07-2P 134135-08-3P 134135-09-4P 134135-10-7P
134135-11-8P 134135-12-9P 134135-13-0P 134135-14-1P 134135-15-2P
134135-16-3P 134135-17-4P 134135-18-5P 134135-19-6P 134135-20-9P
134135-21-0P 134135-22-1P 134135-23-2P 134135-24-3P 134135-25-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as aromatase inhibitor)
IT 134135-40-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for aromatase inhibitor)
IT 21512-16-3P 79387-71-6P 84466-87-5P **112809-25-3P**
112809-54-8P 118618-40-9P 134135-26-5P 134135-27-6P 134135-28-7P
134135-29-8P 134135-30-1P 134135-31-2P 134135-32-3P 134135-33-4P
134135-34-5P 134135-35-6P 134135-36-7P 134135-37-8P 134135-38-9P
134135-39-0P 134135-41-4P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, as intermediate for cycloalkyleneazole aromatase inhibitor)
IT 108-94-1, Cyclohexanone, reactions 120-92-3, Cyclopentanone 288-32-4, Imidazole, reactions 288-88-0, 1H-1,2,4-Triazole 502-42-1, Cycloheptanone 700-58-3, 2-Adamantanone 1066-54-2, Trimethylsilylacetylene 4701-17-1, 5-Bromothiophene-2-carboxaldehyde 17201-43-3, 4-Bromomethylbenzonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of cycloalkyleneazole aromatase inhibitor)
IT **112809-25-3P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, as intermediate for cycloalkyleneazole aromatase inhibitor)

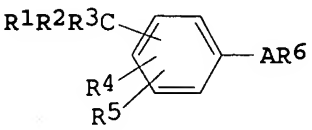
RN 112809-25-3 HCAPLUS
CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)



L52 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:407410 HCAPLUS
DN 111:7410
TI Preparation and formulation of (substituted aralkyl) heterocyclic compounds as aromatase inhibitors
IN Edwards, Philip Neil; Large, Michael Stewart
PA Imperial Chemical Industries PLC, UK
SO Eur. Pat. Appl., 32 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 296749	A1	19881228	EP 1988-305429	19880614
	EP 296749	B1	19941026		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	ZA 8803691	A	19890222	ZA 1988-3691	19880524
	IL 86499	A	19970930	IL 1988-86499	19880525
	AU 8816911	A	19881222	AU 1988-16911	19880531
	AU 605872	B2	19910124		
	US 4935437	A	19900619	US 1988-204743	19880610
	ES 2063036	T3	19950101	ES 1988-305429	19880614
	NO 8802628	A	19881219	NO 1988-2628	19880615
	NO 170080	B	19920601		
	NO 170080	C	19920909		
	CA 1337420	C	19951024	CA 1988-569512	19880615
	DK 8803304	A	19881217	DK 1988-3304	19880616
	DK 174573	B1	20030623		
	FI 8802882	A	19881217	FI 1988-2882	19880616
	FI 97804	B	19961115		
	FI 97804	C	19970225		
	JP 01019067	A	19890123	JP 1988-147068	19880616
	US 36617	E	20000314	US 1996-627311	19960403
PRAI	GB 1987-14013	A	19870616		
	US 1988-204743	A5	19880610		

OS MARPAT 111:7410
GI



I

AB The title compds. [I; R1 = N3, CONH2, cyano, CHO, OH, NO2, 1-hydroxy-C1-6-alkyl, NCCH2CH2, C2-6 alkanoyl, etc.; R2, R3 = H, C1-6 alkyl, halo-C1-6-alkyl, (un)substituted Ph, R2R3 = atoms to complete a 3- to 6-membered ring, etc.; R4 = H, halo, cyano, NO2, C1-6 alkyl, haloalkyl; R5 = MeC(CN)2, F3CSO2, CONH2, pyrrolidinocarbonyl, piperidinocarbonyl, NO2, etc.; A = (un)substituted CH2, CH2CH2, etc.; R6 = 1H-1,2,4-triazol-1-yl, 4H-1,2,4-triazol-1-yl, 1H-imidazol-1-yl, etc.] and their salts, useful as aromatase inhibitors, were prepared 2,2'-(5-Methyl-m-phenylene)bis[2-methylpropionitrile] (preparation given) was brominated with N-bromosuccinimide and the product was was treated with Na triazole to give 2,2'-[5-(1,2,4-triazol-1-ylmethyl)-m-phenylene]bis[2-methylpropionitrile]. I are aromatase inhibitors in vitro at <10 μg/mL, and the preferred I are active at <0.1 μg/mL in vitro and 1.0 mg/kg in vivo, with no toxicity at these doses. Preferred pharmaceutical and veterinary compns. are tablets and capsules containing 0.1-100, preferably 0.25-25 mg I.

IC ICM C07D249-04
ICS C07D233-56; C07D233-90; C07D239-26; C07D213-04; A61K031-41; A61K031-44; A61K031-505

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST aralkyl heterocycle prepn aromatase inhibitor; neoplasm inhibitor aralkyl heterocycle prepn; triazolylmethylphenylenebispropionitrile prepn aromatase inhibitor

IT Neoplasm inhibitors
(substituted aralkylheterocyclic compds.)

IT 443-88-9, 2-Fluoro-m-xylene
RL: RCT (Reactant); RACT (Reactant or reagent)
(Friedel-Crafts acylation of)

IT 676-58-4, Methylmagnesium chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with methylpropionitrile derivative)

IT 109-64-8, 1,3-Dibromopropane 110-52-1, 1,4-Dibromobutane 865-50-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of propionitrile derivative)

IT 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of triazolylbenzoate)

IT 13730-55-7, Methyl 2,5-dimethylbenzoate 25081-39-4, Methyl 3,5-dimethylbenzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)

IT 626-55-1, 3-Bromopyridine 4595-59-9, 5-Bromopyrimidine
RL: RCT (Reactant); RACT (Reactant or reagent)
(**condensation** of, with propionitrile derivative)

IT 19294-04-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of)

IT 9039-48-9, Aromatase
RL: USES (Uses)
(inhibitors, substituted aralkylheterocyclic compds.)

IT 120511-88-8 120512-71-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of)

IT 120511-83-3P 120511-89-9P 120512-25-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and Grignard reaction with methylmagnesium chloride)

IT 120512-38-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and alkylation of)
IT 120512-00-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amination of)
IT 93748-07-3P 120512-51-8P 120512-78-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bromination of)
IT 120511-88-8P 120512-11-0P 120512-19-8P 120512-66-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)
IT 120512-62-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to cyano derivative)
IT 120512-43-8P 120512-60-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion to propionitrile derivative)
IT 27129-86-8P 120511-79-7P 120512-12-1P 120512-36-9P 120512-52-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyanation of)
IT 120512-05-2P 120512-06-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydration of)
IT 120512-17-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydroxylation of)
IT 33016-47-6P 120511-82-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
IT 120512-59-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
IT 120512-40-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and fluorination of)
IT 120511-93-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT 29232-73-3P 39101-54-7P 120511-74-2P 120512-37-0P 120512-45-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
IT 42444-20-2P 120512-13-2P 120512-23-4P 120512-44-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
IT 82594-80-7P, 4-Methyl-1-tritylimidazole
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and quaternization of)
IT 120512-09-6P 120512-20-1P 120532-02-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of)

IT 120511-72-0P 120511-77-5P 120511-78-6P 120511-80-0P 120511-84-4P
120511-86-6P 120511-90-2P 120511-91-3P 120512-02-9P 120512-03-0P
120512-39-2P 120512-41-6P 120512-46-1P 120512-53-0P 120512-54-1P
120512-61-0P 120512-64-3P 120512-68-7P 120512-69-8P 120512-74-5P
120512-76-7P 120512-80-3P 120532-03-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of aromatase inhibitors)

IT 53525-60-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

IT 120511-73-1P 120511-75-3P 120511-76-4P 120511-85-5P 120511-87-7P
120511-92-4P 120511-93-5P 120511-94-6P 120511-95-7P 120511-96-8P
120511-97-9P 120511-98-0P 120511-99-1P 120512-01-8P 120512-04-1P
120512-07-4P 120512-08-5P 120512-10-9P 120512-14-3P
120512-15-4P 120512-16-5P 120512-18-7P 120512-21-2P 120512-22-3P
120512-24-5P 120512-26-7P 120512-27-8P 120512-28-9P 120512-29-0P
120512-30-3P 120512-31-4P 120512-32-5P 120512-33-6P 120512-34-7P
120512-35-8P 120512-47-2P 120512-48-3P 120512-49-4P
120512-50-7P 120512-55-2P 120512-56-3P 120512-57-4P
120512-58-5P 120512-63-2P 120512-65-4P 120512-66-5P 120512-67-6P
120512-70-1P 120512-72-3P 120512-73-4P **120512-75-6P**
120512-77-8P 120512-79-0P 120532-00-5P 120532-01-6P 120532-04-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of, as aromatase inhibitor)

IT 120511-81-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization by, of imidazole derivative)

IT 288-32-4, Imidazole, reactions 288-88-0, 1H-1,2,4-Triazole 41253-21-8, Sodium triazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of aromatase inhibitor)

IT 120511-84-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of aromatase inhibitors)

IT 14527-26-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with propionitrile derivative)

IT 120512-42-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)

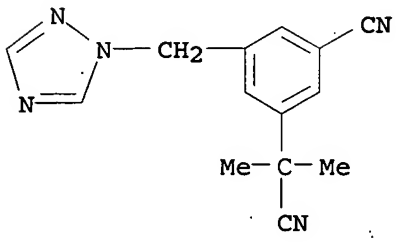
IT 822-36-6, 4-Methylimidazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(tritylation of)

IT 23785-21-9, Ethyl imidazole-4-carboxylate
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-tritylation of)

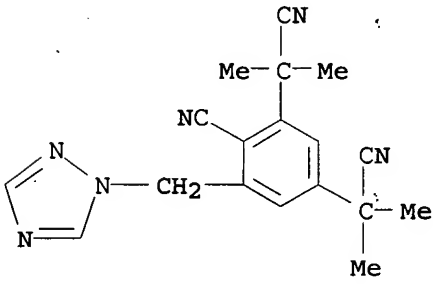
IT **120512-07-4P 120512-50-7P 120512-75-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of, as aromatase inhibitor)

RN 120512-07-4 HCAPLUS
CN Benzeneacetonitrile, 3-cyano-α,α-dimethyl-5-(1H-1,2,4-triazol-

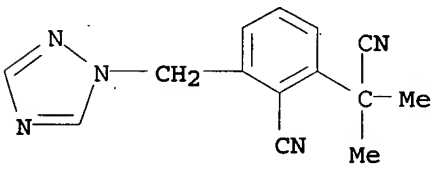
1-ylmethyl)- (9CI) (CA INDEX NAME)



RN 120512-50-7 HCAPLUS
CN 1,3-Benzenediacetonitrile, 4-cyano-α,α,α',α'-tetramethyl-5-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)



RN 120512-75-6 HCAPLUS
CN Benzeneacetonitrile, 2-cyano-α,α-dimethyl-3-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)



L52 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 1988:75402 HCAPLUS
DN 108:75402
TI Preparation and testing of α-heterocyclyltolunitriles as aromatase inhibitors
IN Bowman, Robert Mathews; Steele, Ronald Edward; Browne, Leslie Johnston
PA Ciba-Geigy A.-G. , Switz.
SO Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 236940	A2	19870916	EP 1987-103099	19870305
	EP 236940	A3	19891018		

	EP 236940	B1	19930922		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	US 4749713	A	19880607	US 1986-837489	19860307
	FI 8700903	A	19870908	FI 1987-903	19870302
	FI 91857	B	19940513		
	FI 91857	C	19940825		
	DD 264432	A5	19890201	DD 1987-300415	19870303
	IL 81746	A	19920216	IL 1987-81746	19870303
	HU 43822	A2	19871228	HU 1987-952	19870305
	HU 202843	B	19910429		
	RO 96133	B3	19890130	RO 1987-127283	19870305
	PL 151490	B1	19900928	PL 1987-264460	19870305
	PL 152025	B1	19901031	PL 1987-280247	19870305
	RO 101533	B1	19920625	RO 1987-134372	19870305
	RO 101532	B1	19921103	RO 1987-134373	19870305
	CA 1316928	C	19930427	CA 1987-531185	19870305
	AT 94873	T	19931015	AT 1987-103099	19870305
	ES 2059317	T3	19941116	ES 1987-103099	19870305
	DK 8701176	A	19870908	DK 1987-1176	19870306
	DK 172190	B1	19971222		
	NO 8700937	A	19870908	NO 1987-937	19870306
	NO 170277	B	19920622		
	NO 170277	C	19920930		
	AU 8769768	A	19870910	AU 1987-69768	19870306
	AU 604011	B2	19901206		
	JP 62212369	A	19870918	JP 1987-50446	19870306
	JP 07055930	B	19950614		
	ZA 8701637	A	19871028	ZA 1987-1637	19870306
	SU 1470184	A3	19890330	SU 1987-4202145	19870306
	CZ 279026	B6	19941116	CZ 1987-1512	19870306
	CZ 279027	B6	19941116	CZ 1987-7367	19870306
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	SK 279103	B6	19980603	SK 1987-7368	19871012
	SU 1549478	A3	19900307	SU 1988-4203990	19880118
	SU 1577695	A3	19900707	SU 1988-4203999	19880118
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	EP 1987-103099	A	19870305		

OS CASREACT 108:75402; MARPAT 108:75402

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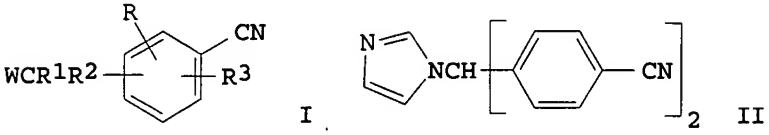

AB The title compds. [I; R, R3 = H, alkyl; adjacent R1R3 = (CH2)4, CH:CHCH:CH; R1, R2 = H, alkenyl, C3-6 cycloalkyl, aryl, R4S, (un)substituted alkyl; R1R2 = (aryl)alkylidene, (alkyl)-C4-6 alkylene, atoms to complete an (un)substituted 5-, 6-, or 7-membered, optionally benzo-fused ring; R4 = alkyl, aryl, aralkyl; W = alkyl-(un)substituted imidazol-1-yl, 1,2,4-triazol-1-yl, 1,2,4-triazol-4-yl, 3-pyridyl] and their pharmaceutically acceptable salts were prepared as aromatase inhibitors, useful in treatment of estrogen-dependent diseases. 4-BrCH2C6H4CN and imidazole were stirred 15 h at room temperature in CH2Cl2 to

give 4-(1H-imidazol-1-ylmethyl)benzonitrile. The latter was stirred at 0-5° with Me3COK in DMF while 4-FC6H4CN in DMF was added dropwise to give methylenebis[benzonitrile] II. I inhibited aromatization of androstenedione in human placental microsomes with IC50 ≥ 10-9 M and inhibited or caused regression of mammary tumors in rats at ≥0.1 mg/kg/day orally. Tablets were prepared containing II hemisuccinate 50.00, lactose 2535.00, cornstarch 125.00, polyethylene glycol 150.00, and Mg stearate 40.00 g per 104.

IC ICM C07D233-56
ICS C07D249-08; C07D213-57; C07D401-04; C07D409-04; A61K031-41; A61K031-415; A61K031-44

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

ST imidazolylmethylbenzonitrile prepn aromatase inhibitor; estrogen inhibitor imidazolylmethylbenzonitrile prepn; neoplasm inhibitor imidazolylmethylbenzonitrile prepn; breast cancer treatment imidazolylmethylbenzonitrile prepn; benzonitrile imidazolylmethyl prepn aromatase inhibitor

IT Neoplasm inhibitors
((imidazolylmethyl)benzonitriles)

IT Estrogens
RL: USES (Uses)
(inhibitors, (imidazolylmethyl)benzonitriles)

IT Mammary gland
(neoplasm, treatment of, (imidazolylmethyl)benzonitriles for)

IT 9039-48-9, Aromatase
RL: USES (Uses)
(inhibitors, (imidazolylmethyl)benzonitriles)

IT 112809-74-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and **condensation** of, with dimethoxybenzophenone)

IT 112809-67-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decomposition of)

IT 13428-06-3P 42252-33-5P 112809-54-8P 112809-55-9P 112809-56-0P
112809-57-1P 112809-58-2P 112809-59-3P 112809-60-6P 112809-61-7P
112809-62-8P 112809-63-9P 112809-64-0P 112809-65-1P 112809-66-2P
112809-68-4P 112809-69-5P 112809-70-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of aromatase inhibitors)

IT 112809-75-3P 112809-76-4P 112809-77-5P 112809-78-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as aromatase inhibitor)

IT 112808-94-3P 112808-95-4P 112808-96-5P 112808-97-6P 112808-98-7P
112808-99-8P 112809-00-4P 112809-01-5P 112809-02-6P 112809-03-7P
112809-04-8P 112809-05-9P 112809-06-0P 112809-07-1P 112809-08-2P
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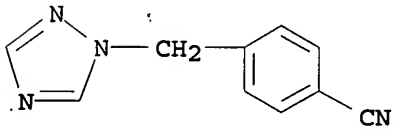
112809-19-5P 112809-20-8P 112809-21-9P 112809-22-0P 112809-23-1P
112809-24-2P **112809-25-3P** **112809-26-4P** 112809-27-5P
112809-28-6P 112809-29-7P 112809-30-0P 112809-31-1P 112809-34-4P
112809-35-5P 112809-36-6P 112809-37-7P 112809-38-8P 112809-39-9P
112809-40-2P 112809-41-3P 112809-42-4P 112809-43-5P 112809-44-6P
112809-45-7P 112809-46-8P 112809-47-9P 112809-48-0P 112809-49-1P
112809-50-4P 112809-51-5P 112809-52-6P 112809-53-7P 112809-71-9P
112809-73-1P 112822-29-4P 133981-86-9P

RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, as estrogen biosynthesis inhibitor)

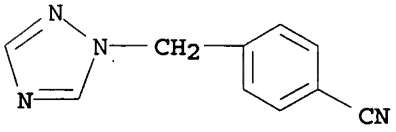
IT 79-44-7, Dimethylcarbamoyl chloride 90-96-0, 4,4'-Dimethoxybenzophenone 104-88-1, 4-Chlorobenzaldehyde, reactions 109-94-4 288-32-4, Imidazole, reactions 288-88-0 612-12-4, α,α'-Dichloro-o-xylene 822-36-6, 4-Methylimidazole 874-86-2, α-Chloro-p-tolunitrile 882-33-7, Diphenyldisulfide 1194-02-1, 4-Fluorobenzonitrile 10297-05-9, 1-Chloro-4-iodobutane 17201-43-3, α-Bromo-p-tolunitrile 30525-89-4, Paraformaldehyde 42498-38-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of aromatase inhibitors)

IT **112809-25-3P 112809-26-4P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, as estrogen biosynthesis inhibitor)

RN 112809-25-3 HCAPLUS
CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

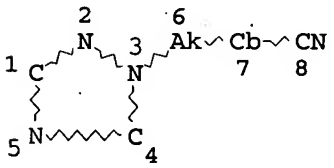


RN 112809-26-4 HCAPLUS
CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

=> => D QUE
L39 STR



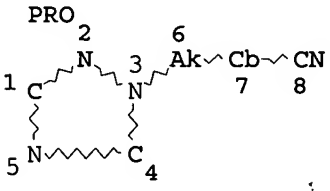
Other preps of the compound

NODE ATTRIBUTES:
CONNECT IS E2 RC AT 6
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 7
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L41 67 SEA FILE=REGISTRY SSS FUL L39
L42 38 SEA FILE=HCAPLUS ABB=ON L41
L43 28 SEA FILE=HCAPLUS ABB=ON L42(L)PREP/RL
L44 1939 SEA FILE=HCAPLUS ABB=ON ?TRIAZOL?(3A)SALT#
L45 1 SEA FILE=HCAPLUS ABB=ON L43 AND L44
L46 8 SEA FILE=HCAPLUS ABB=ON L43 AND CONDENS?
L47 8 SEA FILE=HCAPLUS ABB=ON L45 OR L46
L48 STR



NODE ATTRIBUTES:
CONNECT IS E2 RC AT 6
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 7
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L50 5 SEA FILE=CASREACT SSS FUL L48 (13 REACTIONS)
L51 5 SEA FILE=HCAPLUS ABB=ON L50
L52 5 SEA FILE=HCAPLUS ABB=ON L47 NOT L51
L54 18 SEA FILE=HCAPLUS ABB=ON L43 NOT (L51 OR L52)

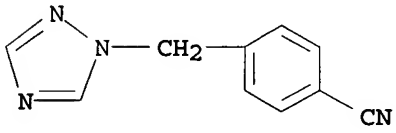
=> D L54 BIB ABS IND HITSTR 1-18

L54 ANSWER 1 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:351870 HCAPLUS
DN 145:124574
TI Process for preparation of letrozole
IN Liu, Kun; Yang, Limin
PA Beijing D-Venturepharm.T. Corp., Peop. Rep. China
SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 7 pp.
CODEN: CNXXEV
DT Patent
LA Chinese
FAN.CNT 1

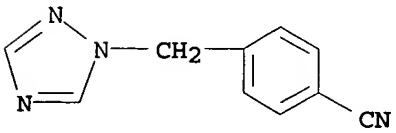
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CN 1754876	A	20060405	CN 2004-10080092	20040928
PRAI	CN 2004-10080092		20040928		

AB This invention relates to a process for preparing letrozole with high purity, which comprises reacting 4-(bromomethyl)benzonitrile with 1,2,4-triazole, separating of the 1,2,4-triazole intermediate from its 1,3,4-isomer, followed by the addition of 4-halo-benzonitrile to give the title compound
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))

ST letrozole prepn triazole
IT Solvents
(water soluble; preparation of letrozole)
IT **112809-25-3P 112809-26-4P 897048-77-0P 897048-78-1P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; preparation of letrozole)
IT 112809-27-5P
RL: BYP (Byproduct); IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of letrozole)
IT **897048-80-5P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of letrozole)
IT 112809-51-5P, Letrozole
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of letrozole)
IT 64-17-5, Ethyl alcohol, uses 67-56-1, Methanol, uses 67-64-1, Acetone, uses 68-12-2, N,N-Dimethyl formamide, uses 75-05-8, Acetonitrile, uses
RL: NUU (Other use, unclassified); USES (Uses)
(preparation of letrozole)
IT 100-47-0D, Benzonitrile, 4-halo 288-88-0, 1H-1,2,4-Triazole 1194-02-1, 4-Fluorobenzonitrile 17201-43-3, 4-Cyano-benzyl-bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of letrozole)
IT **112809-25-3P 112809-26-4P 897048-77-0P 897048-78-1P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; preparation of letrozole)
RN 112809-25-3 HCAPLUS
CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)



RN 112809-26-4 HCAPLUS
CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



O HCl

RN 897048-77-0 HCAPLUS
CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)-, sulfate (1:1) (9CI) (CA INDEX NAME)

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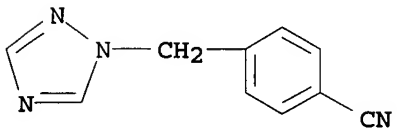
CRN 112809-25-3
CMF C10 H8 N4



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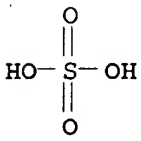
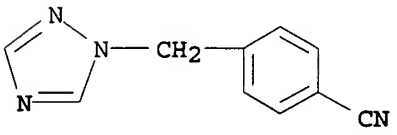
CRN 7664-93-9
CMF H2 O4 S



RN 897048-78-1 HCAPLUS
CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

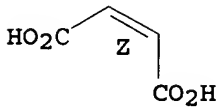
CRN 112809-25-3
CMF C10 H8 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

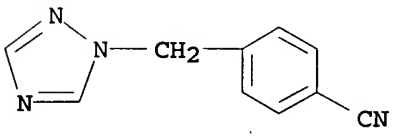
Double bond geometry as shown.



IT **897048-80-5P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of letrozole)
RN 897048-80-5 HCAPLUS
CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)-, monobenzenesulfonate (9CI) (CA INDEX NAME)

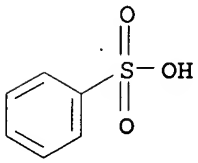
CM 1

CRN 112809-25-3
CMF C10 H8 N4



CM 2

CRN 98-11-3
CMF C6 H6 O3 S



L54 ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:1313847 HCAPLUS
DN 144:51587
TI Preparation of phenyl-sulfamates as aromatase inhibitors
IN Woo, Lok Wai Lawrence; Jackson, Toby; Bubert, Christian; Purohit, Atul; Reed, Michael John; Potter, Barry Victor Lloyd
PA Sterix Limited, UK
SO PCT Int. Appl., 161 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005118560	A1	20051215	WO 2005-GB2194	20050603

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,

CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI GB 2004-12492 A 20040604

OS MARPAT 144:51587

GI For diagram(s), see printed CA Issue.

AB Title compds. represented by the formula I [wherein X, Y, Z = independently an optional liker group; R1 = a ring system; R2 = (oxy)hydrocarbyl, cyano, nitro or halo; R3, R4 = independently H or hydrocarbyl; ring A and B are independently optionally further substituted] were prepared as aromatase inhibitors. For example, II was provided in a multi-step synthesis starting from Me 3,5-dimethylbenzoate. II showed inhibition of aromatase with IC50 value of 3.5 nM.

IC ICM C07D249-08
ICS A61K031-4196; A61P035-00

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

ST phenylsulfamate triazolylmethylphenyl prepn aromatase inhibitor

IT Cell proliferation
(inhibition; preparation of Ph-sulfamates as aromatase inhibitors)

IT Apoptosis
Cell proliferation
Drug delivery systems
(preparation of Ph-sulfamates as aromatase inhibitors)

IT STS (sequence-tagged site)
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of Ph-sulfamates as aromatase inhibitors)

IT 9039-48-9, Aromatase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitor of; preparation of Ph-sulfamates as aromatase inhibitors)

IT 757905-89-8P 871116-59-5P 871116-61-9P 871116-62-0P 871116-64-2P 871116-66-4P 871116-67-5P **871116-69-7P 871116-70-0P** 871116-72-2P 871116-84-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(preparation of Ph-sulfamates as aromatase inhibitors)

IT 120511-73-1P, Anastrozole 871116-60-8P 871116-63-1P 871116-65-3P 871116-68-6P **871116-71-1P** 871116-73-3P 871116-74-4P 871116-75-5P 871116-76-6P 871116-77-7P 871116-78-8P 871116-79-9P 871116-80-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of Ph-sulfamates as aromatase inhibitors)

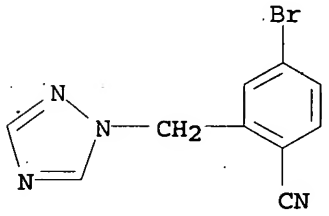
IT 78-75-1, 1,2-Dibromopropane 95-56-7, 2-Bromophenol 99-27-4, 5-Aminoisophthalic acid dimethyl ester 103-16-2, 4-(Benzyloxy)phenol 106-93-4, 1,2-Dibromoethane 108-95-2, Phenol, reactions 288-88-0, 1H-1,2,4-Triazole 556-96-7, 5-Bromo-m-xylene 594-09-2, Trimethylphosphine 624-75-9, Iodoacetonitrile 1486-50-6, 4-Benzyloxybenzoyl chloride 1955-46-0, 5-Nitroisophthalic acid monomethyl ester 2628-17-3, 4-Vinylphenol 7778-42-9, Sulfamoyl

chloride 25081-39-4, Methyl 3,5-dimethylbenzoate 28193-34-2 41253-21-8 67832-11-5, 4-Bromo-2-methylbenzonitrile 71597-85-8, 4-Hydroxyphenylboronic acid 87001-32-9, 4-Benzyloxybenzenesulfonyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of Ph-sulfamates as aromatase inhibitors)

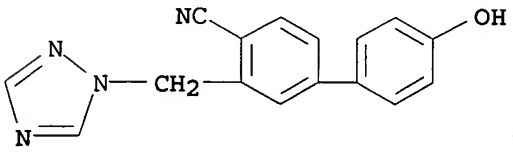
IT 825-90-1P 1955-04-0P 29232-73-3P 29333-41-3P 42843-99-2P 51719-69-8P 53732-08-4P 62262-84-4P 66952-59-8P 66952-60-1P 69332-67-8P 69497-82-1P 77154-19-9P 120511-79-7P 120511-80-0P 120511-81-1P 120511-88-8P 120511-91-3P 120512-11-0P 120512-41-6P 120512-42-7P 142320-39-6P 457051-12-6P 733708-25-3P 757151-49-8P 871116-81-3P 871116-82-4P 871116-83-5P 871116-85-7P 871116-86-8P 871116-87-9P 871116-88-0P 871116-89-1P 871116-90-4P 871116-91-5P 871116-92-6P 871116-93-7P 871116-94-8P 871116-95-9P 871116-96-0P 871116-97-1P 871116-98-2P 871116-99-3P 871117-00-9P 871117-01-0P 871117-02-1P 871117-03-2P 871117-04-3P 871117-05-4P 871117-06-5P 871117-07-6P 871117-08-7P 871117-09-8P 871117-10-1P 871117-11-2P 871117-12-3P 871117-13-4P 871117-14-5P 871117-15-6P 871117-16-7P 871117-17-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of Ph-sulfamates as aromatase inhibitors)

IT **871116-69-7P 871116-70-0P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(preparation of Ph-sulfamates as aromatase inhibitors)

RN 871116-69-7 HCAPLUS
CN Benzonitrile, 4-bromo-2-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)



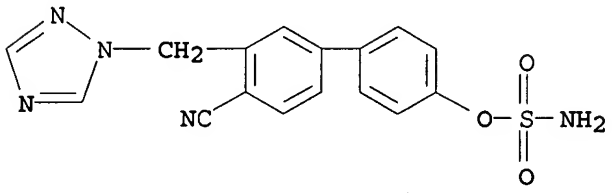
RN 871116-70-0 HCAPLUS
CN [1,1'-Biphenyl]-4-carbonitrile, 4'-hydroxy-3-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)



IT **871116-71-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of Ph-sulfamates as aromatase inhibitors)

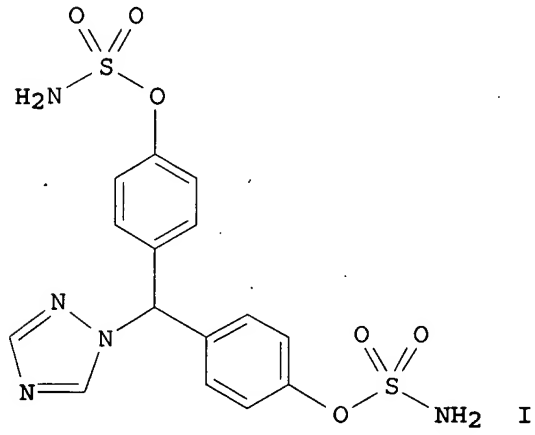
RN 871116-71-1 HCAPLUS

CN Sulfamic acid, 4'-cyano-3'-(1H-1,2,4-triazol-1-ylmethyl)[1,1'-biphenyl]-4-yl ester (9CI) (CA INDEX NAME)

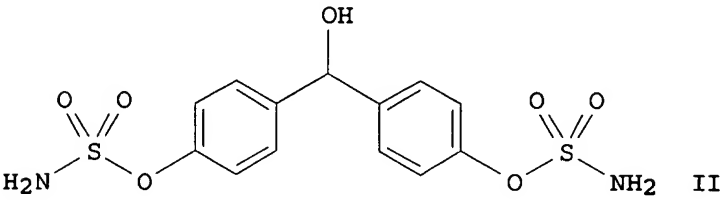


RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:386709 HCAPLUS
DN 143:109140
TI A letrozole-based dual aromatase-sulphatase inhibitor with in vivo activity
AU Wood, Paul M.; Woo, L. W. Lawrence; Humphreys, Anna; Chander, Surinder K.; Purohit, Atul; Reed, Michael J.; Potter, Barry V. L.
CS Medicinal Chemistry, Department of Pharmacy and Pharmacology and Sterix Ltd., University of Bath, Bath, BA2 7AY, UK
SO Journal of Steroid Biochemistry and Molecular Biology (2005), 94(1-3), 123-130
CODEN: JSBBEZ; ISSN: 0960-0760
PB Elsevier B.V.
DT Journal
LA English
GI



I



II

AB The role of aromatase inhibitors in the treatment of hormone-dependent breast cancer is well established. However, it is now recognized that steroid sulfatase (STS) inhibitors represent a new form of endocrine therapy. To explore the potential advantage of dual inhibition by a single agent, we recently developed a series of dual aromatase-sulfatase inhibitors (DASIs) based on the aromatase inhibitor YM511. We report here a new structural class of DASI obtained by obtained introducing the pharmacophore for STS inhibition, i.e. a phenol sulfamate ester into another established aromatase inhibitor letrozole. Hence, the bis-sulfamate (I) was synthesized which exhibited IC50 values of 3044 nM for aromatase and >10 μM for STS in JEG-3 cells. However, at a single oral dose of 10 mg/kg, I inhibited aromatase and rat liver STS by 60% and 88%, resp., 24 h after administration. A proposed metabolite of I, carbinol (II), was synthesized. Despite also showing weak STS inhibition in JEG-3 cells, II inhibited rat liver STS activity to the same extent as I at a single oral dose of 10 mg/kg. Thus, the concept of a letrozole-based DASI has been validated and could be further developed and modified for therapeutic exploitation.

CC 1-6 (Pharmacology)
Section cross-reference(s): 2

ST letrozole aromatase sulphatase inhibitor antitumor breast cancer

IT Antitumor agents
Human
Mammary gland, neoplasm
(letrozole-based dual aromatase-sulfatase inhibitor with in vivo activity)

IT Enzyme inhibitors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(letrozole-based dual aromatase-sulfatase inhibitor with in vivo activity)

IT 9025-62-1, Steroid Sulfatase 9039-48-9, Aromatase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(letrozole-based dual aromatase-sulfatase inhibitor with in vivo activity)

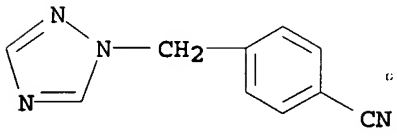
IT 112809-51-5P, Letrozole 537683-34-4P, 1-[Bis-(4-sulphamoyloxyphenyl)methyl]-1H-[1,2,4]triazole 857678-49-0P, Bis-(4-sulphamoyloxyphenyl)methanol
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(letrozole-based dual aromatase-sulfatase inhibitor with in vivo activity)

IT 288-88-0, 1H-1,2,4-Triazole 611-99-4, 4,4'-Dihydroxybenzophenone 29104-30-1, Benzomate
RL: RCT (Reactant); RACT (Reactant or reagent)
(letrozole-based dual aromatase-sulfatase inhibitor with in vivo activity)

IT 40076-84-4P, Bis-(4-benzyloxyphenyl)methanone **112809-25-3P**, 4-1-(1,2,4-Triazolyl)-methyl-benzonitrile 536975-31-2P, Bis-(4-benzyloxyphenyl)methanol 536975-32-3P, 1-[Bis-(4-benzyloxyphenyl)methyl]-1H-[1,2,4]triazole 537677-78-4P, 1-[Bis-(4-hydroxyphenyl)methyl]-1H-[1,2,4]triazole
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(letrozole-based dual aromatase-sulfatase inhibitor with in vivo activity)

IT **112809-25-3P**, 4-1-(1,2,4-Triazolyl)-methyl-benzonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(letrozole-based dual aromatase-sulfatase inhibitor with in vivo

activity)
RN 112809-25-3 HCAPLUS
CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)



RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 4 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:624098 HCAPLUS
DN 142:373269
TI Product class 19: azomethine imines
AU Schantl, J. G.
CS Germany
SO Science of Synthesis (2004), 27, 731-824
CODEN: SSCYJ9
PB Georg Thieme Verlag
DT Journal; General Review
LA English
AB A review. Methods for preparing azomethine imines and their application to organic synthesis.
CC 21-0 (General Organic Chemistry)
ST review azomethine imine prepn org synthesis
IT Imines
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(azomethine; preparation and application of azomethine imines to organic synthesis)
IT 76-05-1, uses 101-83-7 109-63-7 110-86-1, Pyridine, uses 144-55-8, Carbonic acid monosodium salt, uses 497-19-8, Carbonic acid disodium salt, uses 507-40-4 557-34-6 917-54-4 3144-16-9, Camphorsulfonic acid 7440-02-0, Nickel, uses 7440-18-8, Ruthenium, uses 7560-83-0 7732-18-5, Water, uses 15956-28-2 16940-66-2 74735-07-2 312732-34-6
RL: CAT (Catalyst use); USES (Uses)
(preparation and application of azomethine imines to organic synthesis)
IT 50-00-0, Formaldehyde, reactions 60-34-4 66-77-3, 1-Naphthalenecarboxaldehyde 74-99-7, 1-Propyne 75-09-2, reactions 75-15-0, Carbon disulfide, reactions 77-76-9 78-84-2 79-19-6, Hydrazinecarbothioamide 80-17-1 80-62-6 80-63-7 83-38-5 86-81-7 90-02-8, reactions 96-22-0, 3-Pentanone 98-01-1, 2-Furancarboxaldehyde, reactions 98-03-3, 2-Thiophenecarboxaldehyde 98-86-2, reactions 99-61-6 100-06-1 100-10-7 100-16-3 100-34-5 100-42-5, reactions 100-52-7, Benzaldehyde, reactions 100-63-0 102-04-5 103-02-6 103-71-9, reactions 103-72-0 103-79-7 104-15-4, reactions 104-53-0, Benzenepropanal 107-13-1, 2-Propenenitrile, reactions 108-24-7 108-59-8 108-94-1, Cyclohexanone, reactions 108-95-2, Phenol, reactions 111-66-0, 1-Octene 111-78-4, 1,5-Cyclooctadiene 115-11-7, reactions 122-57-6 123-08-0 123-11-5, reactions 123-72-8, Butanal 126-98-7 135-02-4 149-73-5 151-50-8, Potassium cyanide (K(CN)) 272-94-6, 2H-Benzimidazole 333-20-0 333-27-7 334-88-3 446-52-6 455-19-6 462-95-3 463-51-4, Ethenone 487-68-3 498-60-2, 3-Furancarboxaldehyde

500-22-1, 3-Pyridinecarboxaldehyde 513-81-5 536-40-3 536-74-3
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606-26-8 613-94-5 615-13-4 619-27-2 622-36-6 622-82-2 623-47-2
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9-Anthracenecarboxaldehyde 670-54-2, Ethenetetracarbonitrile, reactions
673-32-5 705-31-7 762-42-5 764-42-1 766-91-6 774-48-1 830-79-5
838-14-2 870-46-2 870-50-8 874-42-0 886-38-4 920-37-6 922-67-8
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32064-67-8 33107-14-1 33608-73-0 34899-90-6 36331-57-4
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54856-83-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and application of azomethine imines to organic synthesis)

IT 56077-27-1 57883-13-3 58364-79-7 58645-08-2 59130-82-4
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256658-45-4 256658-49-8 257882-80-7 289909-33-7 298213-97-5
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426829-05-2 433301-93-0 476208-10-3 478488-38-9 596122-91-7
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RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and application of azomethine imines to organic synthesis)

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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and application of azomethine imines to organic synthesis)

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RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and application of azomethine imines to organic synthesis)

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RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and application of azomethine imines to organic synthesis)

IT 596815-11-1P 596815-12-2P 596815-13-3P 596815-14-4P 596815-15-5P
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848651-93-4P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and application of azomethine imines to organic synthesis)

IT **848651-73-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and application of azomethine imines to organic synthesis)

RN 848651-73-0 HCAPLUS
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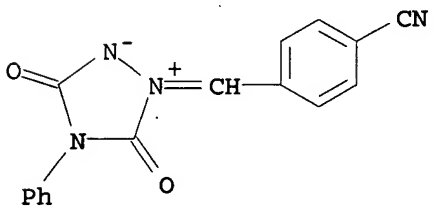

RE.CNT 106 THERE ARE 106 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 5 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 2003:396864 HCAPLUS
DN 138:401733
TI Preparation of triazole derivatives as fungicides
IN Setsu, Fumihito; Umemura, Eijirou; Sasaki, Kazue; Tadauchi, Kaori; Okutomi, Takafumi; Ohtsuka, Keiko; Takahata, Shou
PA Meiji Seika Kaisha, Ltd., Japan
SO PCT Int. Appl., 345 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003042188	A1	20030522	WO 2002-JP11960	20021115
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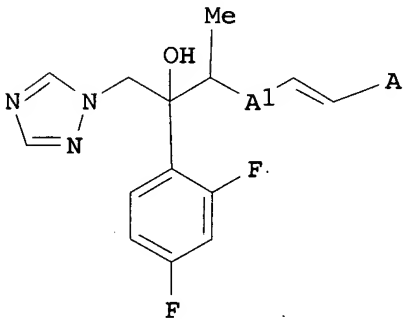
PRAI	JP 2001-349783	A	20011115		

OS MARPAT 138:401733
GI



I

AB The title compds. I [A represents substituted Ph or a 5- to 7-membered, (un)saturated, optionally substituted heterocyclic group; said Ph may be substituted by substituted C1-6 alkyl, optionally substituted sulfonyl, a 5- to 7-membered, (un)saturated, carbocyclic or heterocyclic group, etc.; A1 is (CH2)p; and p is 0 or 1] are prepared Compds. of this invention in vitro showed IC80 of ≤0.0625 μg/mL against C. albicans TIMM1768.

IC ICM C07D249-08
ICS C07D401-10; C07D401-14; C07D403-10; C07D403-14; C07D513-04; C07D413-10; C07D417-10; C07D403-12; A61K031-4196; A61K031-429; A61K031-4439; A61K031-4523; A61K031-454; A61K031-4709; A61K031-4725; A61K031-506; A61K031-5377; A61K031-433; A61K031-422
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 10
ST triazole deriv medical fungicide prepn
IT Aspergillus fumigatus

Mycosis
(candidiasis; preparation and bioeffect of triazole derivs. as fungicides)
IT Fungicides
(medical; preparation of triazole derivs. as fungicides)
IT Mammalia
(preparation and bioeffect of triazole derivs. as fungicides)
IT Mycosis
(preparation of triazole derivs. as fungicides)
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530079-90-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); **PREP (Preparation)**;
USES (Uses)
(preparation of triazole derivs. as fungicides)

IT 530079-91-5P 530079-92-6P 530079-93-7P 530079-94-8P 530079-95-9P
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530080-06-9P 530080-07-0P 530080-08-1P 530080-09-2P 530080-10-5P
530080-11-6P 530080-12-7P 531492-65-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of triazole derivs. as fungicides)

IT 74-88-4, Methyl iodide, reactions 74-89-5, Methylamine, reactions 75-03-6, Iodoethane 75-15-0, Carbon disulfide, reactions 75-30-9, 2-Iodopropane 75-65-0, t-Butanol, reactions 85-41-6, Phthalimide 98-58-8, 4-Bromobenzenesulfonyl chloride 98-88-4, Benzoyl chloride 99-73-0, 4-Bromophenacyl bromide 99-90-1, 4'-Bromoacetophenone 100-39-0, Benzyl bromide 100-46-9, Benzylamine, reactions 104-81-4, α-Bromo-p-xylene 104-95-0, 4-Bromothioanisole 105-36-2, Bromoacetic acid ethyl ester 106-39-8, 1-Bromo-4-chlorobenzene 106-40-1, 4-Bromoaniline 106-53-6, 4-Bromobenzenethiol 107-08-4, 1-Iodopropane 107-20-0, Chloroacetaldehyde 109-97-7, Pyrrole 110-91-8, Morpholine, reactions 124-40-3, Dimethylamine, reactions 137-43-9, Cyclopentyl bromide 149-73-5, Orthoformic acid trimethyl ester 288-13-1, Pyrazole 288-32-4, Imidazole, reactions 288-36-8, 1H-1,2,3-Triazole 288-88-0, 1H-1,2,4-Triazole 288-94-8, 1H-Tetrazole 298-12-4, Glyoxylic acid 332-25-2, 4-Trifluoromethoxybenzonitrile 333-47-1 348-57-2, 1-Bromo-2,4-difluorobenzene 348-61-8, 1-Bromo-3,4-difluorobenzene 353-83-3, 2,2,2-Trifluoroethyl iodide 367-24-8, 4-Bromo-2-fluoroaniline 373-52-4, Bromofluoromethane 392-83-6 393-36-2, 4-Bromo-3-trifluoromethylaniline 393-37-3, 5-Bromo-2-fluorobenzotrifluoride 401-78-5 402-49-3, 4-Trifluoromethylbenzyl bromide 407-14-7, 4-Bromotrifluoromethoxybenzene 445-02-3, 4-Bromo-2-trifluoromethylaniline 455-13-0, 4-Iodobenzotrifluoride 459-46-1, 4-Fluorobenzyl bromide 460-00-4, 1-Bromo-4-fluorobenzene 513-48-4, 2-Iodobutane 540-38-5, 4-Iodophenol 542-69-8, 1-Iodobutane 577-19-5, 1-Bromo-2-nitrobenzene 585-79-5, 1-Bromo-3-nitrobenzene 586-76-5, 4-Bromobenzoic acid 586-77-6, 4-Bromo-N,N-dimethylaniline 586-78-7, 1-Bromo-4-nitrobenzene 589-15-1, 4-Bromobenzyl bromide 591-19-5, 3-Bromoaniline 591-50-4, Iodobenzene 593-56-6, Methoxylamine hydrochloride 615-36-1, 2-Bromoaniline 619-42-1, 4-Bromobenzoic acid methyl ester 622-95-7, 4-Chlorobenzyl bromide 623-00-7, 4-Bromobenzonitrile 623-04-1, 4-Aminobenzyl alcohol 624-31-7, 4-Iodotoluene 624-84-0, N-Formylhydrazine 626-55-1, 3-Bromopyridine 645-36-3, 2,2-Diethoxyethylamine 656-65-5, 4-Bromo-3-fluoroaniline 679-87-8, 2,2,3,3-Tetrafluoropropyl iodide 696-62-8, 4-Iodoanisole 698-67-9, 4-Bromobenzamide 701-34-8, 4-Bromobenzenesulfonamide 707-60-8, N,N-Dimethyl-4-Bromobenzenesulfonamide 766-11-0, 5-Bromo-2-fluoropyridine 824-94-2, 4-Methoxybenzyl chloride 834-66-2 834-67-3 1072-85-1, 1-Bromo-2-fluorobenzene 1072-97-5, 2-Amino-5-bromopyridine 1073-06-9, 1-Bromo-3-fluorobenzene 1133-80-8, 2-Bromofluorene 1193-72-2, 1-Bromo-2,4-dichlorobenzene 1532-97-4, 4-Bromoisoquinoline 1592-00-3, 2-Bromophenyl isocyanate 1730-25-2, Allylmagnesium bromide 1826-67-1, Vinylmagnesium bromide 1885-14-9, Phenyl chloroformate 2052-06-4 2417-72-3, Methyl 4-(bromomethyl)benzoate 2493-02-9, 4-Bromophenyl isocyanate 2537-48-6, Diethyl(cyanomethyl)phosphonate 2746-25-0, 4-Methoxybenzyl bromide 3446-90-0, 4-(Methylthio)benzyl alcohol 3473-63-0, Formamidine acetate 3972-65-4, 1-Bromo-4-t-butylbenzene 4595-59-9, 5-Bromopyrimidine 4648-54-8, Azidotrimethylsilane 4916-55-6, 3-(Bromomethyl)pyridine hydrobromide 5332-24-1, 3-Bromoquinoline 5332-25-2, 6-Bromoquinoline 5470-11-1, Hydroxylamine hydrochloride 5905-69-1 7120-13-0, 6-(4-Bromophenyl)imidazo[2,1-

b]thiazole 7496-46-0, 8-(Bromomethyl)quinoline 7664-41-7, Ammonia, reactions 10075-50-0, 5-Bromoindole 17201-43-3, 4-Cyanobenzyl bromide 19524-06-2, 4-Bromopyridine hydrochloride 21402-26-6, 4-Bromo-3-chloroaniline 23138-55-8, 3-Bromophenyl isocyanate 23915-07-3, 2,4-Difluorobenzyl bromide 26386-88-9, Diphenylphosphoryl azide 26628-22-8, Sodium azide 31106-82-8, 2-Bromomethylpyridine hydrobromide 32315-10-9, Triphosgene 35037-73-1, 4-Trifluoromethoxyphenyl isocyanate 35590-37-5, 3-Bromo-5-cyanopyridine 38762-41-3, 4-Bromo-2-chloroaniline 40161-54-4, 4-Bromo-3-fluorobenzotrifluoride 40161-55-5 40753-13-7, 4-(4-Bromophenyl)-1,2,3-thiadiazole 50709-33-6 50824-05-0, 4-Trifluoromethoxybenzyl bromide 50907-23-8, 5-(4-Bromophenyl)-1H-tetrazole 50998-17-9, 6-Bromoquinoxaline 51376-06-8 51776-71-7 52727-57-8, 2-Amino-5-bromobenzoic acid methyl ester 55661-33-1, 2-Aminomethylthiazole 58479-61-1 66176-39-4, 4-(Bromomethyl)benzenesulfonyl chloride 67567-26-4, 4-Bromo-2,6-difluoroaniline 68834-05-9 72571-06-3 73870-24-3, 4-Bromomethylpyridine hydrobromide 85118-01-0, 3,4-Difluorobenzyl bromide 88112-75-8, 4-Bromo-2-fluorophenyl isocyanate 89226-13-1 103962-10-3, 4-(Trifluoromethoxy)phenacyl bromide 105942-08-3, 4-Bromo-2-fluorobenzonitrile 105942-09-4, 4-Bromomethyl-3-fluorobenzonitrile 127000-90-2 135484-83-2 136350-52-2 138526-69-9, 1-Bromo-3,4,5-trifluorobenzene 151411-98-2, 2,4,6-Trifluorobenzyl bromide 163798-92-3, 4-(4-(Bromomethyl)phenyl)-1,2,3-thiadiazole 175204-45-2, 4-(Bromomethyl)-2,6-dichloropyridine 175278-09-8, 4-Bromo-2-trifluoromethoxyaniline 179897-89-3, 5-Bromo-2-fluorobenzonitrile 213203-65-7, 3-Fluoro-4-trifluoromethylbenzyl bromide 214209-98-0 214210-30-7 239087-07-1 530081-57-3 530081-58-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of triazole derivs. as fungicides)

IT 312-20-9P, 1-Bromo-4-trifluoromethylsulfonylbenzene 703-12-8P 2646-26-6P 5044-39-3P 6188-23-4P 10040-96-7P, 1-(4-Bromophenyl)-1H-imidazole 10075-52-2P, 5-Bromo-1-methylindole 13788-92-6P, 1-(4-Bromophenyl)-1H-pyrazole 18469-37-9P, 4-Bromo-N,N-dimethylbenzamide 20320-17-6P 26197-93-3P 27466-83-7P, 4-Bromo-N-methylbenzamide 30483-75-1P, 4-(4-Bromophenyl)morpholine 38185-19-2P, 4-(Methylthio)benzyl bromide 40724-47-8P, 4-(Bromomethyl)benzenesulfonamide 57058-01-2P, 1-(4-Bromophenyl)-1H-tetrazole 65697-41-8P 69746-31-2P, 5-(p-Bromophenyl)-1-methyltetrazole 74733-90-7P 78838-13-8P 98556-14-0P 111657-87-5P 118863-62-0P 155431-78-0P 161803-04-9P, 4-tert-Butyldiphenylsiloxymethylaniline 161888-38-6P 170230-23-6P 190199-37-2P 197074-69-4P 296796-44-6P 309737-83-5P 425379-95-9P, 1-(5-Bromo-2-fluorophenyl)-1H-pyrazole 433922-57-7P 476194-10-2P 477775-44-3P 513068-89-8P 530080-13-8P 530080-14-9P 530080-15-0P 530080-16-1P 530080-17-2P 530080-18-3P 530080-19-4P 530080-20-7P 530080-21-8P 530080-22-9P 530080-23-0P 530080-24-1P 530080-25-2P 530080-26-3P 530080-27-4P 530080-28-5P 530080-29-6P 530080-30-9P 530080-31-0P 530080-32-1P 530080-33-2P 530080-34-3P 530080-35-4P 530080-36-5P 530080-37-6P 530080-38-7P 530080-39-8P 530080-40-1P 530080-41-2P 530080-42-3P 530080-43-4P 530080-44-5P 530080-45-6P 530080-46-7P 530080-47-8P 530080-48-9P 530080-49-0P 530080-50-3P 530080-51-4P 530080-52-5P 530080-53-6P 530080-54-7P 530080-55-8P 530080-56-9P 530080-57-0P 530080-58-1P 530080-59-2P 530080-60-5P 530080-61-6P 530080-62-7P 530080-63-8P 530080-64-9P 530080-65-0P 530080-66-1P 530080-67-2P 530080-68-3P 530080-69-4P 530080-70-7P 530080-71-8P 530080-72-9P 530080-73-0P 530080-74-1P 530080-75-2P 530080-76-3P 530080-77-4P 530080-78-5P 530080-79-6P 530080-80-9P 530080-81-0P 530080-82-1P 530080-83-2P 530080-84-3P 530080-85-4P 530080-86-5P 530080-87-6P 530080-88-7P

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RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of triazole derivs. as fungicides)

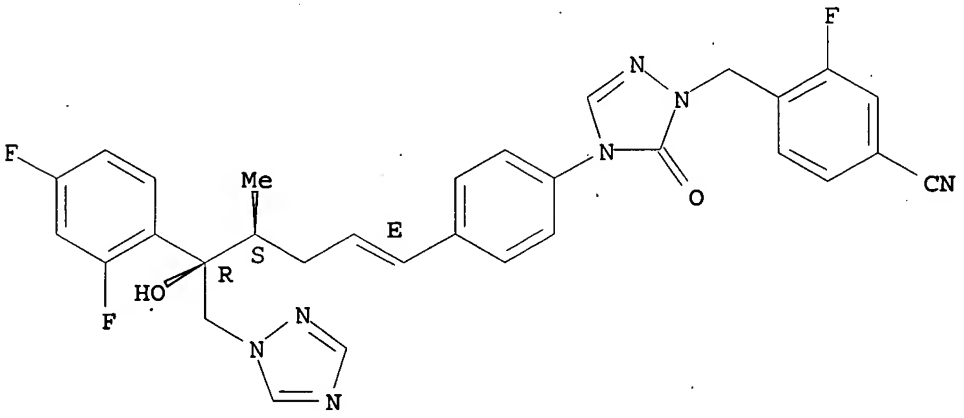
IT **530079-35-7P 530079-69-7P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of triazole derivs. as fungicides)

RN 530079-35-7 HCAPLUS

CN Benzonitrile, 4-[[4-[4-[(1E,4S,5R)-5-(2,4-difluorophenyl)-5-hydroxy-4-methyl-6-(1H-1,2,4-triazol-1-yl)-1-hexenyl]phenyl]-4,5-dihydro-5-oxo-1H-1,2,4-triazol-1-yl]methyl]-3-fluoro- (9CI) (CA INDEX NAME)

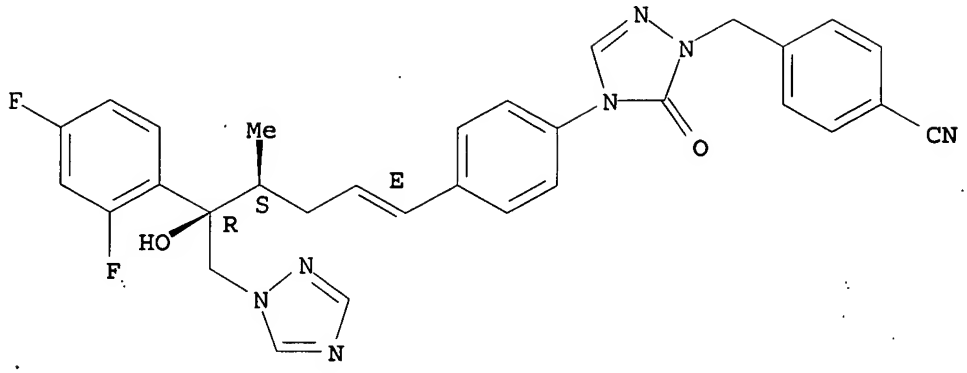
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



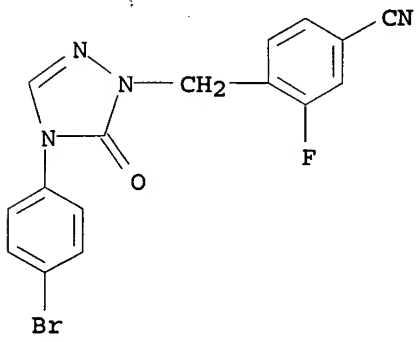
RN 530079-69-7 HCAPLUS

CN Benzonitrile, 4-[[4-[4-[(1E,4S,5R)-5-(2,4-difluorophenyl)-5-hydroxy-4-methyl-6-(1H-1,2,4-triazol-1-yl)-1-hexenyl]phenyl]-4,5-dihydro-5-oxo-1H-1,2,4-triazol-1-yl]methyl]- (9CI) (CA INDEX NAME)

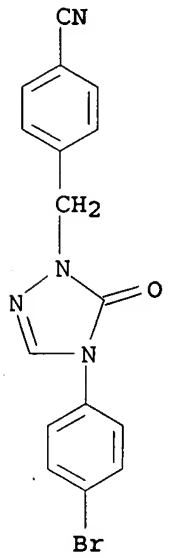
Absolute stereochemistry.
Double bond geometry as shown.



IT **530081-09-5P 530081-48-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of triazole derivs. as fungicides)
RN 530081-09-5 HCAPLUS
CN Benzonitrile, 4-[[4-(4-bromophenyl)-4,5-dihydro-5-oxo-1H-1,2,4-triazol-1-yl]methyl]-3-fluoro- (9CI) (CA INDEX NAME)



RN 530081-48-2 HCAPLUS
CN Benzonitrile, 4-[[4-(4-bromophenyl)-4,5-dihydro-5-oxo-1H-1,2,4-triazol-1-yl]methyl]- (9CI) (CA INDEX NAME)



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:790230 HCAPLUS
DN 137:294961
TI Preparation of 3,5-bishydroxyphenyl-1,2,4-triazoles as pharmaceutical chelators.
IN Lattmann, Rene; Acklin, Pierre
PA Novartis AG, Switz.
SO U.S., 16 pp., Cont.-in-part of U.S. Ser. No. 202,769, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6465504	B1	20021015	US 2000-699765	20001030
	WO 9749395	A1	19971231	WO 1997-EP3315	19970624
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 2003069273	A1	20030410	US 2002-252899	20020923
	US 6596750	B2	20030722		
	US 2003203954	A1	20031030	US 2003-447922	20030529
	US 6723742	B2	20040420		
PRAI	CH 1996-1593	A	19960625		
	WO 1997-EP3315	W	19970624		
	US 1998-202769	B2	19981221		
	US 2000-699765	A3	20001030		
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OS MARPAT 137:294961

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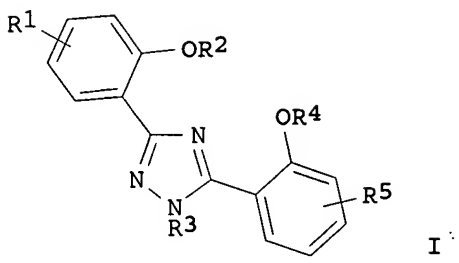


I

AB Title compds. [I; R1, R5 = H, halo, OH, alkyl, haloalkyl, alkoxy, haloalkoxy, CO2H, carbamoyl, alkylcarbamoyl, dialkylcarbamoyl, cyano; R2, R4 = H, (substituted) alkanoyl, aroyl, residue removable under physiol. conditions; R3 = H, alkyl, hydroxyalkyl, haloalkyl, carboxyalkyl, alkoxycarbonylalkyl, (substituted) carbamoyl, aryl, aralkyl, heteroaryl, heteroarylalkyl; with provisos], were prepared Thus, salicyloyl chloride and salicylamide were mixed and heated at 170° to give 2-(2-hydroxyphenyl)benz[e][1,3]oxazin-4-one. The latter was refluxed with 2-hydroxyethylhydrazine in MeOH to give 3,5-bis(2-hydroxyphenyl)-1-(2-hydroxyethyl)-1H-1,2,4-triazole. This at 100 mg/kg in rats gave 368 μg total induced Fe excretion/kg body weight

IC ICM A61K043-653
ICS C07D249-08

INCL 514383000

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST hydroxyphenyltriazole prepn medical chelator; triazole bishydroxyphenyl prepn medical chelator; iron excess treatment diphenyltriazole medical chelator

IT Chelating agents
(medical; preparation of bishydroxyphenyltriazoles as pharmaceutical chelators)

IT Human
(preparation of bishydroxyphenyltriazoles as pharmaceutical chelators)

IT 7439-89-6, Iron, biological studies
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(medical chelating agents for iron; preparation of bishydroxyphenyltriazoles as pharmaceutical chelators)

IT 201530-34-9P, 1H-1,2,4-Triazole-1-ethanol, 3,5-bis(2-hydroxyphenyl)- 201530-36-1P, 1H-1,2,4-Triazole-1-acetic acid, 3,5-bis(2-hydroxyphenyl)-, ethyl ester 201530-38-3P, Phenol, 2,2'-[1-(2,2,2-trifluoroethyl)-1H-1,2,4-triazole-3,5-diyl]bis- 201530-40-7P, Phenol, 2,2'-[1-(4-nitrophenyl)-1H-1,2,4-triazole-3,5-diyl]bis- 201530-41-8P, Benzoic acid, 4-[3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]- 201530-43-0P, Morpholine, 4-[4-[3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]benzoyl]- 201530-44-1P, Piperazine, 1-[4-[3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]benzoyl]-4-methyl- 201530-45-2P, Phenol, 2,2'-[1-(4-methoxyphenyl)-1H-1,2,4-triazole-3,5-diyl]bis- 201530-46-3P, Phenol, 2,2'-[1-(2,4-difluorophenyl)-1H-1,2,4-triazole-3,5-diyl]bis- 201530-47-4P, Phenol, 2,2'-[1-(phenylmethyl)-1H-1,2,4-triazole-3,5-diyl]bis- **201530-48-5P**, Benzonitrile, 4-[[3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]methyl]- 201530-49-6P, Phenol, 2,2'-[1-[[4-(diethylamino)phenyl]methyl]-1H-1,2,4-triazole-3,5-diyl]bis- 201530-50-9P, Phenol, 2,2'-[1-[[4-(1-pyrrolidinyl)phenyl]methyl]-1H-1,2,4-triazole-3,5-diyl]bis- 201530-51-0P, Phenol, 2,2'-[1-(4-pyridinylmethyl)-

1H-1,2,4-triazole-3,5-diyl]bis- 201530-52-1P, Phenol, 2,2'-[1-(3-pyridinylmethyl)-1H-1,2,4-triazole-3,5-diyl]bis- 201530-53-2P, 1H-1,2,4-Triazole-1-ethanol, 3,5-bis(5-chloro-2-hydroxyphenyl)- 201530-54-3P, Benzoic acid, 4-[3,5-bis(5-chloro-2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]- 201530-55-4P, Phenol, 2,2'-[1-(2-pyridinylmethyl)-1H-1,2,4-triazole-3,5-diyl]bis[4-chloro- 201530-56-5P, Phenol, 2,2'-[1-[[4-(dimethylamino)phenyl]methyl]-1H-1,2,4-triazole-3,5-diyl]bis[4-chloro- 201530-57-6P, Benzoic acid, 4-[3,5-bis(5-fluoro-2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]- 201530-58-7P, Benzoic acid, 4-[3,5-bis(2-hydroxy-5-methylphenyl)-1H-1,2,4-triazol-1-yl]- 201530-59-8P, 1H-1,2,4-Triazole-1-acetic acid, 3,5-bis(2-hydroxyphenyl)- 201530-60-1P, 1H-1,2,4-Triazole-1-acetamide, 3,5-bis(2-hydroxyphenyl)-N-methyl- 201530-61-2P, 1H-1,2,4-Triazole-1-acetamide, N-(2-hydroxyethyl)-3,5-bis(2-hydroxyphenyl)- 201530-62-3P, 1H-1,2,4-Triazole-1-acetamide, 3,5-bis(2-hydroxyphenyl)-N-(2-methoxyethyl)- 201530-63-4P, 1H-1,2,4-Triazole-1-acetamide, N-(2,3-dihydroxypropyl)-3,5-bis(2-hydroxyphenyl)- 201530-64-5P, 1H-1,2,4-Triazole-1-acetamide, 3,5-bis(2-hydroxyphenyl)-N-[2-(4-morpholinyl)ethyl]- 201530-65-6P, 1H-1,2,4-Triazole-1-acetamide, N-(2-hydroxyethyl)-3,5-bis(2-hydroxyphenyl)-N-methyl- 201530-66-7P, 1H-1,2,4-Triazole-1-acetamide, N-[2-(2-hydroxyethoxy)ethyl]-3,5-bis(2-hydroxyphenyl)- 201530-67-8P, 1H-1,2,4-Triazole-1-acetamide, N-[2-[bis(2-hydroxyethyl)amino]ethyl]-3,5-bis(2-hydroxyphenyl)- 201530-68-9P, 1H-1,2,4-Triazole-1-acetamide, N-[2-hydroxy-1-(hydroxymethyl)ethyl]-3,5-bis(2-hydroxyphenyl)- 201530-69-0P, 1H-1,2,4-Triazole-1-acetamide, 3,5-bis(2-hydroxyphenyl)-N-[2-(4-methyl-1-piperazinyl)ethyl]- 201530-70-3P, 1H-1,2,4-Triazole-1-acetamide, 3,5-bis(2-hydroxyphenyl)-N,N-dimethyl- 201530-71-4P, Morpholine, 4-[[3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]acetyl]- 201530-72-5P, Piperazine, 1-[[3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]acetyl]-4-methyl- 201530-73-6P, 1H-1,2,4-Triazole-1-acetamide, 3,5-bis(2-hydroxyphenyl)-N-methyl-N-(phenylmethyl)- 201530-74-7P, 1H-1,2,4-Triazole-1-acetamide, N,N-bis(2-hydroxyethyl)-3,5-bis(2-hydroxyphenyl)- 201530-75-8P, 1H-1,2,4-Triazole-1-acetamide, N-[2-(dimethylamino)ethyl]-3,5-bis(2-hydroxyphenyl)-N-methyl- 201530-76-9P, 1H-1,2,4-Triazole-1-acetamide, 3,5-bis(5-chloro-2-hydroxyphenyl)-N-[2-(4-morpholinyl)ethyl]- 201530-77-0P, 1H-1,2,4-Triazole-1-acetic acid, 3,5-bis(5-chloro-2-hydroxyphenyl)-, ethyl ester 201530-78-1P, Benzoic acid, 2-[3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]- 201530-79-2P, Benzoic acid, 4-[3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]-, ethyl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of bishydroxyphenyltriazoles as pharmaceutical chelators)

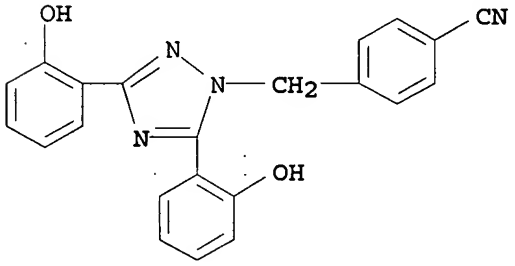
IT 65-45-2, Salicylamide 103-67-3, N-Methylbenzylamine 109-01-3, 1-Methylpiperazine 109-83-1, N-Methylethanolamine 109-84-2, 2-Hydroxyethylhydrazine 109-85-3, 2-Methoxyethylamine 110-91-8, Morpholine, reactions 111-42-2, Ethanol, 2,2'-iminobis-, reactions 141-43-5, Ethanol, 2-amino-, reactions 142-25-6, N,N,N'-Trimethylethylenediamine 321-14-2, Benzoic acid, 5-chloro-2-hydroxy- 345-16-4, 5-Fluorosalicylic acid 534-03-2, 2-Amino-1,3-propanediol 616-30-8, 3-Amino-1,2-propanediol 619-67-0, 4-Hydrazinobenzoic acid 870-46-2, tert-Butyl carbazate 929-06-6, 2-(2-Aminoethoxy)ethanol 934-98-5, 1-Piperazineethanamine, 4-methyl- 1073-62-7, Benzylhydrazine hydrochloride 1441-87-8, Salicyloyl chloride 2038-03-1, 4-(2-Aminoethyl)morpholine 3197-06-6, Ethanol, 2,2'-[(2-aminoethyl)imino]bis- 5042-30-8, 2,2,2-Trifluoroethylhydrazine 5326-27-2, 2-Hydrazinobenzoic acid 6945-92-2, Ethyl hydrazinoacetate hydrochloride 7120-43-6, Benzamide, 5-chloro-2-hydroxy- 19501-58-7, 4-Methoxyphenylhydrazine hydrochloride 24798-62-7, 4H-1,3-Benzoxazin-4-

one, 2-(2-hydroxy-5-methylphenyl)-6-methyl- 26189-59-3, 1-Propen-1-amine, 1-chloro-N,N,2-trimethyl- 40594-29-4, 2,4-Difluorophenylhydrazine hydrochloride 51980-54-2, 4-Pyrrolidinobenzaldehyde 56413-74-2, 4-Nitrophenylhydrazine hydrochloride 56874-97-6, 5-Fluorosalicylamide 57616-01-0, Pyridine, 3-(hydrazinomethyl)-, monohydrochloride 89598-56-1, Pyridine, 4-(hydrazinomethyl)-, dihydrochloride 201530-83-8, 4-Cyanobenzylhydrazine hydrochloride 201530-84-9, Benzenamine, N,N-diethyl-4-(hydrazinomethyl)-, hydrochloride 201530-85-0, Pyridine, 2-(hydrazinomethyl)-, hydrochloride 201530-86-1, Benzenamine, 4-(hydrazinomethyl)-N,N-dimethyl-, hydrochloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bishydroxyphenyltriazoles as pharmaceutical chelators)

IT 1218-69-5P, 4H-1,3-Benzoxazin-4-one, 2-(2-hydroxyphenyl)- 201530-80-5P, Pyrrolidine, 1-[4-(hydrazinomethyl)phenyl]-, hydrochloride 201530-81-6P, 4H-1,3-Benzoxazin-4-one, 6-chloro-2-(5-chloro-2-hydroxyphenyl)- 201530-82-7P, 4H-1,3-Benzoxazin-4-one, 6-fluoro-2-(5-fluoro-2-hydroxyphenyl)-
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bishydroxyphenyltriazoles as pharmaceutical chelators)

IT **201530-48-5P**, Benzonitrile, 4-[[3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]methyl]-
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of bishydroxyphenyltriazoles as pharmaceutical chelators)

RN 201530-48-5 HCAPLUS
CN Benzonitrile, 4-[[3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]methyl]- (9CI) (CA INDEX NAME)



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 7 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:909664 HCAPLUS
DN 134:56695
TI Procedure for the production of 2-heterocyclylmethylbenzoic acid derivatives
IN Wroblowsky, Heinz-Juergen; Schallner, Otto; Schwarz, Hans-Georg
PA Bayer A.-G., Germany
SO Ger. Offen., 18 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI	DE 19929348	A1	20001228	DE 1999-19929348	19990626
	WO 2001000595	A1	20010104	WO 2000-EP5412	20000613
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	BR 2000012451	A	20020402	BR 2000-12451	20000613
	EP 1194419	A1	20020410	EP 2000-940367	20000613
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2003503396	T	20030128	JP 2001-507005	20000613
	IN 2001MN01533	A	20050401	IN 2001-MN1533	20011205
PRAI	DE 1999-19929348	A	19990626		
	WO 2000-EP5412	W	20000613		

OS MARPAT 134:56695

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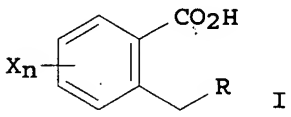


I

AB Title compds. I [R = N-heterocyclyl attached through N; X = NO2, CN, CONH2, CSNH2, halogen, (un)substituted alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, NH2, H2NSO2; n = 0-3] were prepared by treating phthalides with the N heterocycles. Thus, 4-methyl-5-trifluoromethyl-2,4-dihydro-3H-1,2,4-triazol-3-one was converted to its K salt and treated with phthalide to give 74% I [n = 0, R = 4-methyl-3-trifluoromethyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-1-yl]. The compds. are synthetic intermediates.

IC ICM C07D249-12
ICS C07D237-32; C07D253-08; C07D263-58; C07D235-26; C07D233-84; C07D213-64; C07D521-00

CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))

ST heterocyclylmethylbenzoic acid prepn; benzoic acid heterocyclylmethyl prepn

IT 87-41-2, Phthalide 51856-10-1 53065-38-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(procedure for the production of 2-heterocyclylmethylbenzoic acid derivs.)

IT 313474-86-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(procedure for the production of 2-heterocyclylmethylbenzoic acid derivs.)

IT 55207-90-4P 256232-25-4P 256232-26-5P 256232-27-6P 256232-28-7P
256232-29-8P 256232-32-3P 256232-33-4P 256232-34-5P 256232-41-4P
256232-47-0P 256232-60-7P 256232-62-9P 256232-69-6P 256232-70-9P
256232-78-7P 256232-83-4P 256232-85-6P 256232-86-7P 256232-87-8P
256232-88-9P 313474-88-3P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(procedure for the production of 2-heterocyclylmethylbenzoic acid derivs.)

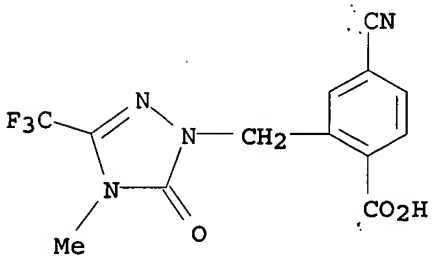
IT 256232-84-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(two tautomers; procedure for the production of 2-heterocyclylmethylbenzoic acid derivs.)

IT **256232-88-9P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(procedure for the production of 2-heterocyclylmethylbenzoic acid derivs.)

RN 256232-88-9 HCAPLUS

CN Benzoic acid, 4-cyano-2-[[4,5-dihydro-4-methyl-5-oxo-3-(trifluoromethyl)-1H-1,2,4-triazol-1-yl]methyl]- (9CI) (CA INDEX NAME)



L54 ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 2000:785840 HCAPLUS

DN 133:350223

TI Preparation of dioxoalkylbenzyltriazolones and related compounds as herbicides.

IN Mueller, Klaus-Helmut; Lehr, Stefan; Schallner, Otto; Schwarz, Hans-Georg; Wroblowsky, Heinz-Juergen; Drewes, Mark Wilhelm; Feucht, Dieter; Pontzen, Rolf; Wetcholowsky, Ingo

PA Bayer A.-G., Germany

SO Ger. Offen., 82 pp.
CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19921424	A1	20001109	DE 1999-19921424	19990508
	IN 2000MU00366	A	20050304	IN 2000-MU366	20000419
	CA 2373076	A1	20001116	CA 2000-2373076	20000426
	WO 2000068204	A1	20001116	WO 2000-EP3712	20000426
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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	EP 1181280	B1	20041201		
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	BR 2000010388	A	20020319	BR 2000-10388	20000426
	JP 2002544198	T	20021224	JP 2000-617184	20000426
	AU 764182	B2	20030814	AU 2000-45563	20000426
	AT 283842	T	20041215	AT 2000-927048	20000426
	RU 2245330	C2	20050127	RU 2001-133347	20000426

	ES 2235868	T3	20050716	ES 2000-927048	20000426
	US 6762152	B1	20040713	US 2001-9981	20011105
PRAI	DE 1999-19921424	A	19990508		
	WO 2000-EP3712	W	20000426		

OS MARPAT 133:350223

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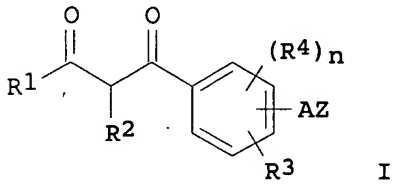

I

AB Title compds. [I; n = 0-3; A = bond, alkylene; R1 = H, (substituted) alkyl, cycloalkyl; R2 = H, cyano, carbamoyl, halo, (substituted) alkyl, alkoxy, alkoxycarbonyl, alkylthio, alkylsulfinyl, alkylsulfonyl; R3 = H, NO2, cyano, CO2H, carbamoyl, thiocarbamoyl, halo, (substituted) alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, dialkylamino, dialkylaminosulfonyl; R4 = NO2, cyano, CO2H, carbamoyl, thiocarbamoyl, halo, (substituted) alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, dialkylamino, dialkylaminosulfonyl; Z = (substituted) 4-12 membered mono- or bicyclic heterocyclyl containing ≤4 N atoms and 1-3 CO or CS groups], were prepared as herbicides (no data). Thus, 4-cyclopropyl-5-ethoxy-2-(2-carboxy-5-trifluoromethylbenzyl)-2,4-dihydro-3H-1,2,4-triazol-3-one in DMF was treated with cyanomethyl cyclopropyl ketone (preparation given), Et3N, and di-Et cyanophosphonate followed by stirring for 2 days to give 40% 3-cyclopropyl-2-[2-[4-(cyclopropyl-3-ethoxy-5-oxo-4,5-dihydro-1H-1,2,4-triazol-1-yl)methyl]-4-trifluoromethylbenzoyl]-3-oxopropanenitrile.

IC ICM C07D249-12
ICS C07D285-12; C07D247-00; C07D227-02; C07D255-00; C07D269-00; C07D283-00; C07D487-04; C07D471-04; A01N043-00; A01N053-04

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

ST dioxoalkylbenzyltriazolone prepn herbicide; triazolone cyclopropylcyanodioxopropylbenzyl prepn herbicide

IT Herbicides
(preparation of dioxoalkylbenzyltriazolones as herbicides)

IT 304904-85-6P 304904-86-7P 304904-87-8P 304904-88-9P 304904-89-0P 304904-90-3P 304904-91-4P 304904-92-5P 304904-93-6P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dioxoalkylbenzyltriazolones as herbicides)

IT 75-05-8, Acetonitrile, reactions 2868-37-3, Methyl cyclopropanecarboxylate 135280-73-8 256232-94-7 304904-95-8 304904-96-9 304904-97-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of dioxoalkylbenzyltriazolones as herbicides)

IT 55207-90-4P 118431-88-2P 256231-75-1P 256231-76-2P 256231-78-4P 256231-79-5P 256231-80-8P 256231-81-9P 256231-82-0P 256231-83-1P 256231-84-2P 256231-85-3P 256231-86-4P 256231-87-5P 256231-88-6P 256231-89-7P 256231-90-0P 256231-91-1P 256231-92-2P 256231-93-3P

256231-94-4P 256231-95-5P 256231-96-6P 256231-97-7P 256231-98-8P
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256232-10-7P 256232-11-8P 256232-12-9P 256232-13-0P 256232-14-1P
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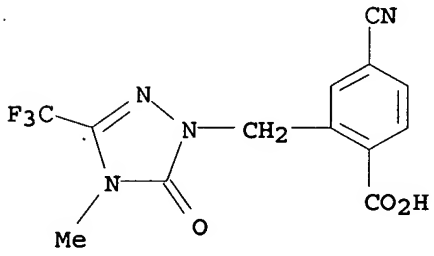
256232-45-8P 256232-46-9P 256232-47-0P 256232-48-1P 256232-49-2P
256232-50-5P 256232-51-6P 256232-52-7P 256232-53-8P 256232-54-9P
256232-55-0P 256232-56-1P 256232-57-2P 256232-58-3P 256232-59-4P
256232-60-7P 256232-61-8P 256232-62-9P 256232-63-0P 256232-64-1P
256232-65-2P 256232-66-3P 256232-67-4P 256232-68-5P 256232-69-6P
256232-70-9P 256232-71-0P 256232-72-1P 256232-73-2P 256232-74-3P
256232-75-4P 256232-76-5P 256232-77-6P 256232-78-7P 256232-79-8P
256232-80-1P 256232-81-2P 256232-82-3P 256232-83-4P 256232-84-5P
256232-85-6P 256232-86-7P 256232-87-8P **256232-88-9P**
295797-06-7P 304904-94-7P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of dioxoalkylbenzyltriazolones as herbicides)

IT **256232-88-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of dioxoalkylbenzyltriazolones as herbicides)

RN 256232-88-9 HCAPLUS
CN Benzoic acid, 4-cyano-2-[[4,5-dihydro-4-methyl-5-oxo-3-(trifluoromethyl)-1H-1,2,4-triazol-1-yl]methyl]- (9CI) (CA INDEX NAME)



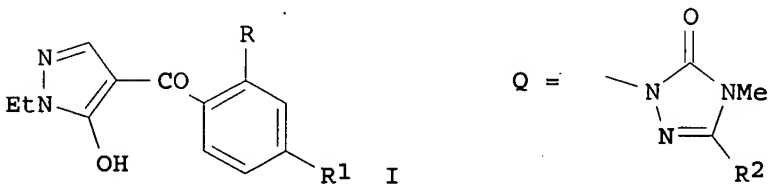
L54 ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:686146 HCAPLUS
DN 133:252427
TI Preparation of herbicidal benzoylpyrazoles
IN Mueller, Klaus-Helmut; Lehr, Stefan; Schallner, Otto; Schwarz, Hans-Georg; Wroblowsky, Heinz-Juergen; Drewes, Mark Wilhelm; Feucht, Dieter; Pontzen, Rolf; Wetcholowsky, Ingo
PA Bayer A.-G., Germany
SO Ger. Offen., 108 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19914140	A1	20000928	DE 1999-19914140	19990327

	CA 2368459	A1	20001005	CA 2000-2368459	20000315
	WO 2000058306	A1	20001005	WO 2000-EP2292	20000315
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	BR 2000009389	A	20011226	BR 2000-9389	20000315
	EP 1165547	A1	20020102	EP 2000-912609	20000315
	EP 1165547	B1	20030827		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2002540205	T	20021126	JP 2000-608008	20000315
	AT 248164	T	20030915	AT 2000-912609	20000315
	ES 2200844	T3	20040316	ES 2000-912609	20000315
	RU 2242465	C2	20041220	RU 2001-129149	20000315
	IN 2001MN01108	A	20050304	IN 2001-MN1108	20010913
	US 6746989	B1	20040608	US 2001-937631	20010926
	US 2004248740	A1	20041209	US 2004-768322	20040130
PRAI	DE 1999-19914140	A	19990327		
	WO 2000-EP2292	W	20000315		
	US 2001-937631	A3	20010926		

OS MARPAT 133:252427

GI



AB Benzoylpyrazole derivs., such as I [R = Cl, R1 = Q, R2 = CF3; R = CH2Q, R1 = CF3, R2 = OEt, SMe], were prepared for use as herbicides (no data). Thus, the triazolylbenzoyl chloride was treated with 1-ethyl-5-pyrazolol to give I [R = Cl, R1 = Q, R2 = CF3].

IC ICM C07D403-10
ICS A01N043-56; A01N043-653

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

ST triazolylbenzoylpyrazole prepn herbicide; benzoylpyrazole triazolyl triazolylalkyl prepn herbicide; pyrazole triazolylbenzoyl triazolylalkylbenzoyl prepn herbicide

IT Herbicides
(preparation of herbicidal benzoylpyrazoles)

IT 295796-72-4P 295796-73-5P 295796-74-6P 295796-75-7P 295796-76-8P
295796-77-9P 295796-78-0P 295796-79-1P 295796-80-4P 295796-81-5P
295796-82-6P 295796-83-7P 295796-84-8P 295796-85-9P 295796-86-0P
295796-87-1P 295796-88-2P 295796-89-3P 295796-90-6P 295796-91-7P
295796-92-8P 295796-93-9P 295796-95-1P 295796-96-2P 295796-97-3P
295796-98-4P

RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of herbicidal benzoylpyrazoles)

IT 22354-80-9 23984-82-9, 2-Methyl-4-trifluoromethylbenzoic acid
256231-75-1 256232-95-8 295797-37-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of herbicidal benzoylpyrazoles)

IT 55207-90-4P 256231-76-2P 256231-77-3P 256231-78-4P 256231-79-5P
256231-80-8P 256231-82-0P 256231-83-1P 256231-84-2P 256231-85-3P
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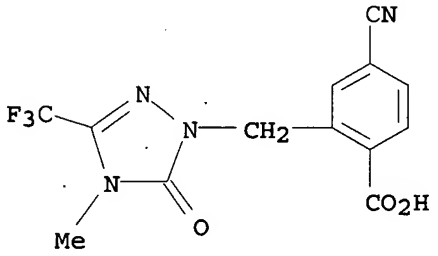
256234-01-2P 256234-02-3P 256234-05-6P 256234-06-7P 256234-07-8P
256234-08-9P 295796-99-5P 295797-00-1P 295797-01-2P 295797-05-6P
295797-06-7P 295797-09-0P 295797-10-3P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of herbicidal benzoylpyrazoles)

IT **256232-88-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)

(preparation of herbicidal benzoylpyrazoles)
RN 256232-88-9 HCAPLUS
CN Benzoic acid, 4-cyano-2-[[4,5-dihydro-4-methyl-5-oxo-3-(trifluoromethyl)-1H-1,2,4-triazol-1-yl]methyl]- (9CI) (CA INDEX NAME)



L54 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:401964 HCAPLUS
DN 133:55325
TI Inhibitors of prenyl-protein transferase and their therapeutic use
IN De Solms, S. Jane; Graham, Samuel L.; Shaw, Anthony W.; Ciccarone, Terrence M.; Stokker, Gerald E.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 281 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000034437	A2	20000615	WO 1999-US29075	19991207
WO 2000034437	A3	20001116		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2000024774	A1	20000626	AU 2000-24774	19991207
US 6284755	B1	20010904	US 1999-456153	19991207
US 2002037888	A1	20020328	US 2001-819522	20010328
PRAI US 1998-111416P	P	19981208		
US 1999-129282P	P	19990414		
US 1999-456153	A3	19991207		
WO 1999-US29075	W	19991207		

OS MARPAT 133:55325
AB The present invention is directed to compds. which inhibit prenyl-protein transferase (FTase) and the prenylation of the oncogene protein Ras. The invention is further directed to chemotherapeutic compns. containing the compds. of this invention and methods for inhibiting prenyl-protein transferase and the prenylation of the oncogene protein Ras. Thus, a large number of inhibitors, such as 4-imidazol-1-ylmethyl-2-[2-(2-oxopiperidin-1-yl)phenoxy]benzonitrile, were synthesized and tested for inhibition of ras farnesyl transferase in vitro. These compds. had IC50's of ≤30 μM.

IC ICM C12N
CC 7-3 (Enzymes)
Section cross-reference(s): 1
ST prenyl protein transferase inhibitor synthesis chemotherapy
IT Blindness
(caused by retinal vascularization; inhibitors of prenyl-protein transferase and their therapeutic use)
IT Hepatitis delta virus
(infections of; inhibitors of prenyl-protein transferase and their therapeutic use)
IT Antitumor agents
(inhibitors of prenyl-protein transferase and their therapeutic use)
IT Disease, animal
(neurofibromen benign proliferative disorder; inhibitors of prenyl-protein transferase and their therapeutic use)
IT Kidney, disease
(polycystic; inhibitors of prenyl-protein transferase and their therapeutic use)
IT Artery, disease
(restenosis; inhibitors of prenyl-protein transferase and their therapeutic use)
IT Eye
(retina, vascularization, blindness caused by; inhibitors of prenyl-protein transferase and their therapeutic use)
IT 198625-84-2 262363-29-1
RL: PRP (Properties)
(Unclaimed; inhibitors of prenyl-protein transferase and their therapeutic use)
IT 275805-76-0P 275805-77-1P 275805-78-2P 275805-79-3P 275805-80-6P
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275805-87-3P 275805-88-4P 275805-89-5P 275805-90-8P 275805-91-9P
275805-92-0P 275805-93-1P 275805-94-2P 275805-95-3P
275805-96-4P 275805-97-5P 275805-98-6P 275805-99-7P 275806-00-3P
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275807-59-5P 275807-60-8P 275807-61-9P 275807-62-0P 275807-63-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(inhibitors of prenyl-protein transferase and their therapeutic use)

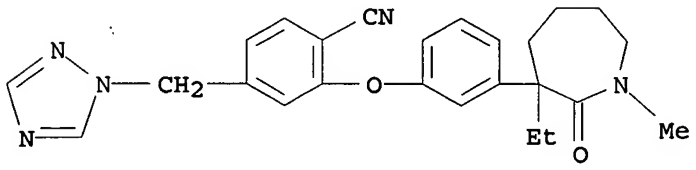
IT 131384-38-8, Farnesyl protein transferase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors of prenyl-protein transferase and their therapeutic use)

IT 51-45-6, Histamine, reactions 75-77-4, reactions 95-55-6, 2-Aminophenol 95-92-1, Diethyl oxalate 105-60-2, reactions 106-95-6, Allyl bromide, reactions 109-04-6, 2-Bromopyridine 109-83-1, N-Methylaminoethanol 110-91-8, Morpholine, reactions 288-32-4, Imidazole, reactions 452-74-4, 4-Bromo-3-fluorotoluene 592-55-2 625-92-3, 3,5-Dibromopyridine 626-55-1, 3-Bromopyridine 762-72-1 766-51-8, 2-Chloroanisole 1005-56-7, Phenyl thionochloroformate 1609-86-5, tert-Butyl isocyanate 2398-37-0, 3-Bromoanisole 2556-73-2, N-Methylcaprolactam 4509-90-4, 5-Bromovaleryl chloride 5470-11-1, Hydroxylamine hydrochloride 10130-74-2, 3-Methoxybenzenesulfonyl chloride 24424-99-5 30525-89-4, Paraformaldehyde 51721-15-4 71556-74-6 77801-57-1 87199-16-4, 3-Formylphenylboronic acid 96797-15-8, 4-Iodo-1-trityl-1H-imidazole 275808-59-8 275808-60-1 275808-61-2 275808-62-3 275808-64-5 275808-66-7 275808-68-9 275808-70-3 275808-72-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(inhibitors of prenyl-protein transferase and their therapeutic use)

IT 3553-94-4P 7624-61-5P 15547-89-4P 27180-90-1P 59263-75-1P 62467-43-0P 67935-17-5P 71556-71-3P 71556-81-5P 71556-83-7P 71592-43-3P 71592-44-4P 76778-37-5P 101048-76-4P 133059-43-5P 153556-42-4P 173681-63-5P 177273-35-7P 222978-01-0P 222978-02-1P 222978-03-2P 222978-04-3P 222978-20-3P 222978-21-4P 222978-22-5P 222978-23-6P 222978-24-7P 222978-25-8P 222978-26-9P 222978-28-1P 222978-29-2P 254451-36-0P 275807-65-3P 275807-66-4P 275807-67-5P 275807-68-6P 275807-69-7P 275807-70-0P 275807-71-1P 275807-72-2P 275807-73-3P 275807-74-4P 275807-75-5P 275807-76-6P 275807-77-7P 275807-78-8P 275807-79-9P 275807-80-2P 275807-81-3P 275807-82-4P 275807-83-5P 275807-84-6P 275807-85-7P 275807-86-8P 275807-87-9P 275807-88-0P 275807-89-1P 275807-90-4P 275807-91-5P 275807-92-6P 275807-93-7P 275807-94-8P 275807-95-9P 275807-96-0P 275807-97-1P 275807-98-2P 275807-99-3P 275808-00-9P 275808-02-1P 275808-04-3P 275808-06-5P 275808-07-6P 275808-08-7P 275808-09-8P 275808-10-1P 275808-11-2P 275808-13-4P 275808-14-5P 275808-16-7P 275808-17-8P 275808-19-0P 275808-20-3P 275808-21-4P 275808-24-7P 275808-25-8P 275808-27-0P 275808-30-5P 275808-32-7P 275808-34-9P 275808-35-0P 275808-36-1P 275808-37-2P 275808-38-3P 275808-39-4P 275808-41-8P 275808-43-0P 275808-44-1P 275808-45-2P 275808-46-3P 275808-48-5P 275808-50-9P 275808-53-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(inhibitors of prenyl-protein transferase and their therapeutic use)

IT 262946-56-5 262946-57-6 262946-58-7 262946-59-8 262946-60-1 262946-61-2 262946-62-3 262946-63-4 262946-64-5 262946-65-6 262946-66-7 262946-67-8 262946-68-9 262946-69-0 262946-70-3 262946-71-4 262946-72-5 262946-73-6 262946-74-7
RL: PRP (Properties)
(unclaimed nucleotide sequence; inhibitors of prenyl-protein transferase and their therapeutic use)

IT **275805-92-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(inhibitors of prenyl-protein transferase and their therapeutic use)
RN 275805-92-0 HCAPLUS
CN Benzonitrile, 2-[3-(3-ethylhexahydro-1-methyl-2-oxo-1H-azepin-3-yl)phenoxy]-4-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)



L54 ANSWER 11 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:161267 HCAPLUS
DN 132:194379
TI Preparation of 1,2,4-triazole-3-thiones for treating a chemokine mediated disease
IN Baxter, Andrew; Bennion, Colin; Cage, Peter; Kindon, Nicholas; Mortimore, Michael; Roberts, Bryan
PA Astra Pharmaceuticals Ltd., UK; Astra Aktiebolag
SO PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000012489	A1	20000309	WO 1999-SE1469	19990827
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9958923	A1	20000321	AU 1999-58923	19990827
	EP 1109790	A1	20010627	EP 1999-946526	19990827
	EP 1109790	B1	20030514		
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	JP 2002525281	T	20020813	JP 2000-571050	19990827
	AT 240303	T	20030515	AT 1999-946526	19990827
	US 2002086862	A1	20020704	US 2001-6245	20011210
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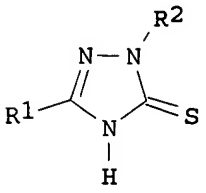
	WO 1999-SE1469	W	19990827		
	US 1999-403419	A1	19991021		

OS MARPAT 132:194379
GI



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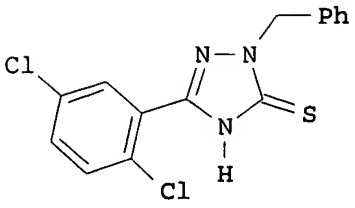

II

AB The title compds. [I; R1 = (un)substituted Ph, naphthyl, 5-6 membered heterocyclic aromatic group containing at least one heteroatom selected from N, O and S; R2 = (un)substituted alkylphenyl], useful in treating a chemokine mediated disease wherein the chemokine binds to a CXCR2 receptor (e.g. in treating an inflammatory disease such as psoriasis), were prepared Thus, treating 2,5-dichlorobenzoic acid with oxalyl chloride and DMF in CH2Cl2 followed by reacting the intermediate with 2-phenylmethylthiosemicarbazide in the presence of pyridine afforded 1,2,4-triazole-3-thione II. Biol. data for compds. I were given.

IC ICM C07D249-12
ICS C07D401-04; C07D405-04; C07D409-04; A61K031-4196

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST triazolethione prepn chemokine mediated disease CXCR2; antiinflammatory triazolethione prepn; psoriasis triazolethione prepn

IT Chemokine receptors
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(CXCR2; preparation of 1,2,4-triazole-3-thiones for treating a chemokine mediated disease)

IT Anti-inflammatory agents
(preparation of 1,2,4-triazole-3-thiones for treating a chemokine mediated disease)

IT Psoriasis
(treatment of; preparation of 1,2,4-triazole-3-thiones for treating a chemokine mediated disease)

IT Interleukin 8 receptors
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(β; preparation of 1,2,4-triazole-3-thiones for treating a chemokine mediated disease)

IT 260056-76-6P 260056-77-7P 260056-78-8P 260056-79-9P 260056-80-2P
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260057-37-2P 260057-38-3P 260057-39-4P **260057-40-7P**
260057-41-8P 260057-42-9P 260057-43-0P 260057-44-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)

(preparation of 1,2,4-triazole-3-thiones for treating a chemokine mediated disease)

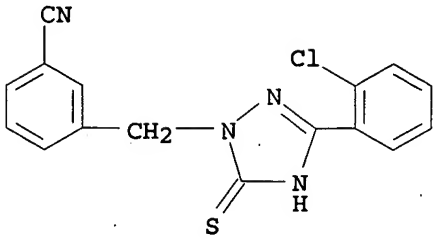
IT 50-79-3, 2,5-Dichlorobenzoic acid 59-67-6, 3-Pyridinecarboxylic acid, reactions 65-85-0, Benzoic acid, reactions 89-75-8, 2,4-Dichlorobenzoyl chloride 99-94-5 100-09-4, 4-Methoxybenzoic acid 100-11-8, 4-Nitrobenzyl bromide 103-63-9, (2-Bromoethyl)benzene 104-81-4, 4-Methylbenzyl bromide 104-88-1, 4-Chlorobenzaldehyde, reactions 118-91-2, 2-Chlorobenzoic acid 122-04-3, 4-Nitrobenzoyl chloride 122-78-1, Phenylacetaldehyde 122-97-4, 3-Phenyl-1-propanol 393-52-2, 2-Fluorobenzoyl chloride 402-49-3, 4-(Trifluoromethyl)benzyl bromide 434-75-3, 2-Chloro-6-fluorobenzoic acid 455-24-3, 4-Trifluoromethylbenzoic acid 456-42-8, 3-Fluorophenylmethyl chloride 527-69-5, 2-Furoyl chloride 532-55-8, Benzoyl isothiocyanate 536-66-3, 4-Isopropylbenzoic acid 555-96-4, Benzylhydrazine 579-18-0, Benzophenone-3-carboxylic acid 586-75-4, 4-Bromobenzoyl chloride 586-76-5, 4-Bromobenzoic acid 587-04-2, 3-Chlorobenzaldehyde 591-31-1, 3-Methoxybenzaldehyde 610-14-0, 2-Nitrobenzoyl chloride 618-46-2, 3-Chlorobenzoyl chloride 620-23-5, 3-Methylbenzaldehyde 874-60-2, 4-Methylbenzoyl chloride 879-18-5, 1-Naphthoyl chloride 933-88-0, 2-Methylbenzoyl chloride 1679-64-7, Mono-methyl terephthalate 2215-77-2, 4-Phenoxybenzoic acid 2243-42-7, 2-Phenoxybenzoic acid 2251-65-2, 3-Trifluoromethylbenzoyl chloride 2252-51-9, 2-Chloro-4-fluorobenzoic acid 2746-25-0, 4-Methoxyphenylmethyl bromide 2905-60-4, 2,3-Dichlorobenzoyl chloride 2905-62-6, 3,5-Dichlorobenzoyl chloride 3024-72-4, 3,4-Dichlorobenzoyl chloride 3724-10-5, 2-Methylthiobenzoic acid 3739-38-6, 3-Phenoxybenzoic acid 4376-18-5, Methyl hydrogen phthalate 5182-44-5, 3-Chlorophenethyl alcohol 5271-67-0, Thiophene-2-carbonyl chloride 6068-72-0, 4-Cyanobenzoyl chloride 7154-66-7, 2-Bromobenzoyl chloride 14002-51-8, 4-Biphenylcarbonyl chloride 16778-84-0, 4-Methoxybenzoyl isothiocyanate 18880-00-7, 4-(1,1-Dimethylethyl)benzyl bromide 20717-79-7, 1-Bromo-2-naphthoic acid 21198-19-6 21615-34-9, 2-Methoxybenzoyl chloride 24065-33-6, 5-Chlorothiophene-2-carboxylic acid 28188-41-2, 3-Bromomethylbenzonitrile 39178-35-3, Isonicotinyl chloride hydrochloride 39515-51-0, 3-Phenoxybenzaldehyde 40400-13-3, 2-Iodobenzyl bromide 40929-48-4, 5-Pyrimidinecarbonyl chloride 49609-84-9, 2-Chloronicotinyl chloride 50837-53-1, 2,5-Dimethylbenzyl bromide 52496-75-0 53874-66-1 56658-04-9, 2-Bromo-5-methoxybenzoyl chloride 57248-14-3, 2,5-Dichlorothiophene-3-carbonyl chloride 58755-00-3 59337-89-2, 3-Chlorothiophene-2-carboxylic acid 85117-99-3, 2,5-Difluorobenzyl bromide 260057-48-5 260057-49-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 1,2,4-triazole-3-thiones for treating a chemokine mediated disease)

IT 260057-45-2P 260057-46-3P 260057-47-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,2,4-triazole-3-thiones for treating a chemokine mediated disease)

IT **260057-40-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of 1,2,4-triazole-3-thiones for treating a chemokine mediated disease)

RN 260057-40-7 HCAPLUS

CN Benzonitrile, 3-[[3-(2-chlorophenyl)-2,5-dihydro-5-thioxo-1H-1,2,4-triazol-1-yl]methyl]- (9CI) (CA INDEX NAME)

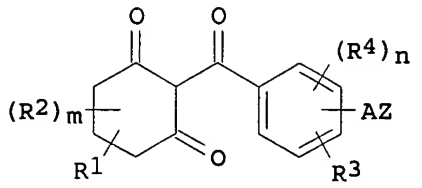


RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:65543 HCAPLUS
DN 132:122623
TI Preparation of 2-(oxotriazolylbenzoyl)-1,3-cyclohexanediones and related compounds as herbicides.
IN Schwarz, Hans-Georg; Mueller, Kläus-Helmut; Lehr, Stefan; Schallner, Otto; Wroblowsky, Heinz-Juergen; Drewes, Mark Wilhelm; Feucht, Dieter; Pontzen, Rolf; Wetcholowsky, Ingo
PA Bayer A.-G., Germany
SO Ger. Offen., 114 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19921732	A1	20000127	DE 1999-19921732	19990511
	IN 1999DE00944	A	20050701	IN 1999-DE944	19990705
	CA 2338304	A1	20000203	CA 1999-2338304	19990713
	WO 2000005221	A1	20000203	WO 1999-EP4929	19990713
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9955050	A	20000214	AU 1999-55050	19990713
	AU 749204	B2	20020620		
	BR 9912392	A	20010508	BR 1999-12392	19990713
	EP 1100789	A1	20010523	EP 1999-941423	19990713
	EP 1100789	B1	20050209		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2002521373	T	20020716	JP 2000-561177	19990713
	AT 288900	T	20050215	AT 1999-941423	19990713
	RU 2248352	C2	20050320	RU 2001-105907	19990713
	ES 2237141	T3	20050716	ES 1999-941423	19990713
	US 6924251	B1	20050802	US 2001-743876	19990713
PRAI	DE 1998-19833360	A1	19980724		
	DE 1999-19921732	A	19990511		
	WO 1999-EP4929	W	19990713		

OS MARPAT 132:122623
GI



I

AB Title compds. [I; m, n = 0-3; A = bond, alkylene; R1 = H, (substituted) alkyl, alkoxycarbonyl; R2 = (substituted) alkyl; R1R2 = alkylene; R3 = H, NO2, cyano, CO2H, carbamoyl, thiocarbamoyl, halo, (substituted) alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, dialkylamino, dialkylaminosulfonyl; R4 = NO2, cyano, CO2H, carbamoyl, thiocarbamoyl, halo, (substituted) alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, dialkylamino, dialkylaminosulfonyl; Z = (substituted) 4-12 membered mono- or bicyclic heterocyclyl], were prepared Thus, 5-ethoxy-4-methyl-2-(2-carboxy-5-trifluoromethylbenzyl)-2,4-dihydro-3H-1,2,4-triazol-3-one, 1,3-cyclohexanedione, and DCC were stirred overnight in MeCN; Et3N and Me3SiCN were added to give after 3 h 52% 5-ethoxy-4-methyl-[2-(2,6-dioxocyclohexylcarbonyl)-5-trifluoromethylbenzyl]2,4-dihydro-3H-1,2,4-triazol-3-one. The latter was said to show strong herbicidal activity combined with good crop tolerance.

IC ICM C07D249-12
ICS C07D227-02; C07D247-00; C07D269-00; C07D255-00; C07D283-00; A01N043-64; C07C049-792

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

ST oxotriazolylbenzoylcyclohexanedione prepn herbicide; cyclohexanedione oxotriazolylbenzoyl prepn herbicide

IT Herbicides
(preparation of 2-(oxotriazolylbenzoyl)-1,3-cyclohexanediones and related compds. as herbicides)

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256412-83-6P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of 2-(oxotriazolylbenzoyl)-1,3-cyclohexanediones and related compds. as herbicides)

IT 504-02-9, 1,3-Cyclohexanedione 22354-80-9 23984-82-9 51856-10-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2-(oxotriazolylbenzoyl)-1,3-cyclohexanediones and related compds. as herbicides)

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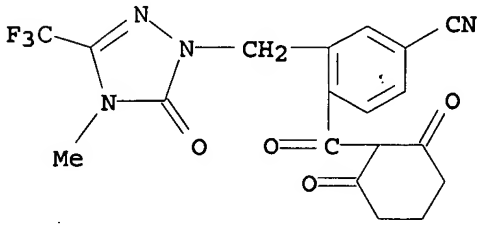
256233-64-4P 256233-65-5P 256233-66-6P 256233-67-7P 256233-68-8P
256233-69-9P 256233-70-2P 256233-71-3P 256233-72-4P 256233-73-5P
256233-74-6P 256233-75-7P 256233-76-8P 256233-77-9P 256233-78-0P
256233-80-4P 256233-81-5P 256233-82-6P 256233-83-7P 256233-84-8P
256233-85-9P 256233-86-0P 256233-87-1P 256233-88-2P 256233-89-3P
256233-90-6P 256233-91-7P 256233-92-8P 256233-93-9P 256233-94-0P
256233-95-1P 256233-96-2P 256233-97-3P 256233-98-4P 256233-99-5P
256234-00-1P 256234-01-2P 256234-02-3P 256234-03-4P 256234-04-5P
256234-05-6P 256234-06-7P 256234-07-8P 256234-08-9P 256234-09-0P
256234-10-3P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**

(Preparation); RACT (Reactant or reagent)
(preparation of 2-(oxotriazolylbenzoyl)-1,3-cyclohexanediones and related compds. as herbicides)

IT **256231-41-1P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of 2-(oxotriazolylbenzoyl)-1,3-cyclohexanediones and related compds. as herbicides)

RN 256231-41-1 HCAPLUS

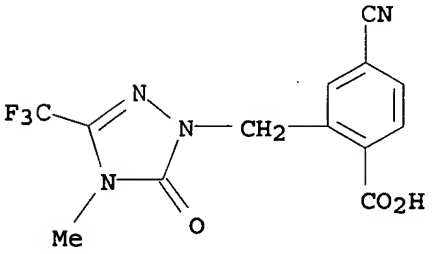
CN Benzonitrile, 3-[[4,5-dihydro-4-methyl-5-oxo-3-(trifluoromethyl)-1H-1,2,4-triazol-1-yl]methyl]-4-[(2,6-dioxocyclohexyl)carbonyl]- (9CI) (CA INDEX NAME)



IT **256232-88-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of 2-(oxotriazolylbenzoyl)-1,3-cyclohexanediones and related compds. as herbicides)

RN 256232-88-9 HCAPLUS

CN Benzoic acid, 4-cyano-2-[[4,5-dihydro-4-methyl-5-oxo-3-(trifluoromethyl)-1H-1,2,4-triazol-1-yl]methyl]- (9CI) (CA INDEX NAME)



L54 ANSWER 13 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 1998:42274 HCAPLUS

DN 128:114953

TI Preparation of substituted 3,5-diphenyl-1,2,4-triazoles as pharmaceutical metal chelators.

IN Lattmann, Rene; Acklin, Pierre

PA Novartis A-G., Switz.

SO PCT Int. Appl., 43 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9749395	A1	19971231	WO 1997-EP3315	19970624
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	TW 533205	B	20030521	TW 1997-86108750	19970623
	CA 2255951	A1	19971231	CA 1997-2255951	19970624
	CA 2255951	C	20061010		
	AU 9732629	A	19980114	AU 1997-32629	19970624
	AU 718037	B2	20000406		
	EP 914118	A1	19990512	EP 1997-928269	19970624
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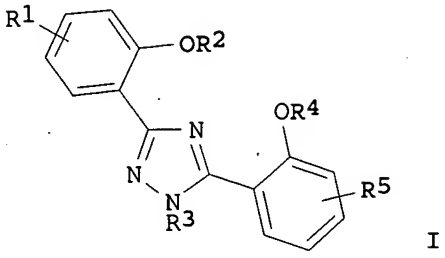
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	CN 1223579	A	19990721	CN 1997-195831	19970624
	BR 9709973	A	19990810	BR 1997-9973	19970624
	HU 9903111	A2	20000128	HU 1999-3111	19970624
	NZ 333308	A	20000526	NZ 1997-333308	19970624
	JP 2000507601	T	20000620	JP 1998-502348	19970624
	JP 3541042	B2	20040707		
	AT 226435	T	20021115	AT 1997-928269	19970624
	AP 1127	A	20021206	AP 1998-1407	19970624
	W: GH, KE, SZ, ZW				
	PT 914118	T	20030228	PT 1997-928269	19970624
	CZ 291470	B6	20030312	CZ 1998-4272	19970624
	ES 2187785	T3	20030616	ES 1997-928269	19970624
	RU 2208010	C2	20030710	RU 1999-101050	19970624
	SK 284319	B6	20050103	SK 1998-1785	19970624
	BG 64248	B1	20040730	BG 1998-103003	19981208
	NO 9806024	A	19981221	NO 1998-6024	19981221
	NO 317180	B1	20040906		
	KR 2000022222	A	20000425	KR 1998-710642	19981224
	HK 1020530	A1	20030613	HK 1999-105147	19991109
	US 6465504	B1	20021015	US 2000-699765	20001030
	US 2003069273	A1	20030410	US 2002-252899	20020923
	US 6596750	B2	20030722		
	US 2003203954	A1	20031030	US 2003-447922	20030529
	US 6723742	B2	20040420		
PRAI	CH 1996-1593	A	19960625		
	WO 1997-EP3315	W	19970624		
	US 1998-202769	B2	19981221		
	US 2000-699765	A3	20001030		
	US 2002-252899	A3	20020923		
OS	MARPAT 128:114953				
GI					



I

AB Title compds. [I; R1, R5 = H, halo, OH, alkyl, haloalkyl, alkoxy, haloalkoxy, CO2H, carbamoyl, alkylcarbamoyl, dialkylcarbamoyl, cyano; R2, R4 = H, (substituted) alkanoyl, aroyl, residue removable under physiol. conditions; R3 = H, alkyl, hydroxyalkyl, haloalkyl, carboxyalkyl, alkoxycarbonylalkyl, (substituted) carbamoyl, aryl, aralkyl, heteroaryl, heteroarylalkyl], were prepared for treatment of diseases involving excess iron (no data). Thus, salicyloyl chloride and salicylamide were mixed and heated at 170° to give 2-(2-hydroxyphenyl)benz[e][1,3]oxazin-4-one. The latter was refluxed with 2-hydroxyethylhydrazine in MeOH to give 3,5-bis(2-hydroxyphenyl)-1-(2-hydroxyethyl)-1H-1,2,4-triazole.

IC ICM A61K031-41
ICS C07D249-08; C07D401-06

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST phenyltriazole prepn medical chelator; triazole diphenyl prepn medical chelator; iron excess treatment diphenyltriazole medical chelator

IT Chelating agents
(medical; preparation of substituted 3,5-diphenyl-1,2,4-triazoles as pharmaceutical metal chelators)

IT 7439-89-6, Iron, biological studies
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(medical chelating agents for iron; preparation of substituted 3,5-diphenyl-1,2,4-triazoles as pharmaceutical metal chelators)

IT 201530-34-9P 201530-36-1P 201530-38-3P 201530-40-7P 201530-41-8P
201530-43-0P 201530-44-1P 201530-45-2P 201530-46-3P 201530-47-4P
201530-48-5P 201530-49-6P 201530-50-9P 201530-51-0P
201530-52-1P 201530-53-2P 201530-54-3P 201530-55-4P 201530-56-5P
201530-57-6P 201530-58-7P 201530-59-8P 201530-60-1P 201530-61-2P
201530-62-3P 201530-63-4P 201530-64-5P 201530-65-6P 201530-66-7P
201530-67-8P 201530-68-9P 201530-69-0P 201530-70-3P 201530-71-4P
201530-72-5P 201530-73-6P 201530-74-7P 201530-75-8P 201530-76-9P
201530-77-0P 201530-78-1P 201530-79-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of substituted 3,5-diphenyl-1,2,4-triazoles as pharmaceutical metal chelators)

IT 65-45-2, Salicylamide 103-67-3, N-Methylbenzylamine 109-01-3, 1-Methylpiperazine 109-83-1, N-Methylethanolamine 109-84-2, 2-Hydroxyethylhydrazine 109-85-3, 2-Methoxyethylamine 110-91-8, Morpholine, reactions 111-42-2, reactions 141-43-5, reactions 321-14-2 345-16-4, 5-Fluorosalicylic acid 534-03-2, 2-Amino-1,3-propanediol 616-30-8, 3-Amino-1,2-propanediol 619-67-0, 4-Hydrazinobenzoic acid 870-46-2, tert-Butyl carbazate 929-06-6, 2-(2-Aminoethoxy)ethanol 934-98-5 1441-87-8, Salicyloyl chloride 2038-03-1, 4-(2-Aminoethyl)morpholine 3197-06-6 5042-30-8, 2,2,2-Trifluoroethylhydrazine 5326-27-2, 2-Hydrazinobenzoic acid

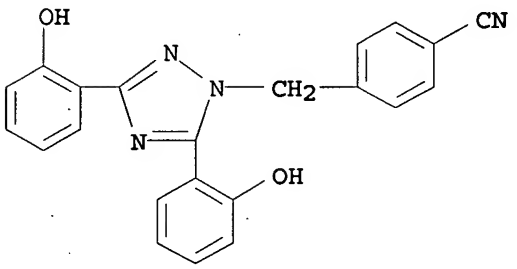
6945-92-2, Ethyl hydrazinoacetate hydrochloride 7120-43-6 19501-58-7, 4-Methoxyphenylhydrazine hydrochloride 24798-62-7 26189-59-3 40594-29-4, 2,4-Difluorophenylhydrazine hydrochloride 51980-54-2, 4-Pyrrolidinobenzaldehyde 56413-74-2, 4-Nitrophenylhydrazine hydrochloride 56874-97-6, 5-Fluorosalicylamide 57616-01-0 89598-56-1 201530-83-8, 4-Cyanobenzylhydrazine hydrochloride 201530-84-9 201530-85-0 201530-86-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted 3,5-diphenyl-1,2,4-triazoles as pharmaceutical metal chelators)

IT 1218-69-5P 201530-80-5P 201530-81-6P 201530-82-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted 3,5-diphenyl-1,2,4-triazoles as pharmaceutical metal chelators)

IT **201530-48-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of substituted 3,5-diphenyl-1,2,4-triazoles as pharmaceutical metal chelators)

RN 201530-48-5 HCAPLUS

CN Benzonitrile, 4-[[3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]methyl]- (9CI) (CA INDEX NAME)



L54 ANSWER 14 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 1996:150244 HCAPLUS

DN 124:202271

TI Novel azolyl methyl phenyl derivatives having aromatase inhibitory activity.

IN Murakami, Kimihiro; Ohnishi, Shuhei; Yano, Takashi; Itoh, manabu

PA Mochida Pharmaceutical Co., Ltd., Japan

SO Eur. Pat. Appl., 60 pp.
CODEN: EPXXDW

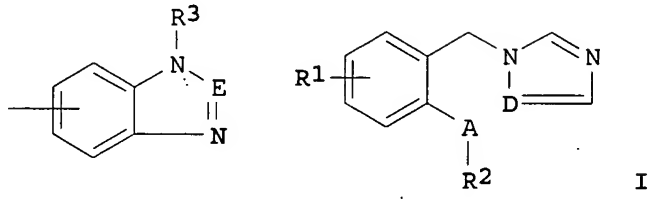
DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 684235	A1	19951129	EP 1995-108053	19950526
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 08041032	A	19960213	JP 1995-122690	19950522
	CA 2150326	A1	19951128	CA 1995-2150326	19950526
	AU 9520332	A	19951207	AU 1995-20332	19950526
	AU 682947	B2	19971023		

US 5587392 A 19961224 US 1995-453054 19950526
PRAI JP 1994-115664 A 19940527
OS MARPAT 124:202271
GI



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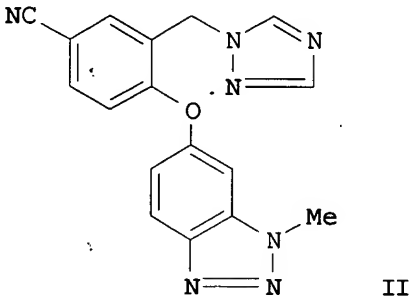


II

AB Compds. I [A = CH2, O, S; D = N, CH; R1 = halo, cyano, NO2, C1-2 (fluoro)alkoxy, (fluoro)alkyl, alkoxycarbonyl, C2-5 alkenyl, alkynyl, CO2H, Ac, CHO, H; R2 = 1- or 2-naphthyl, heterocyclic group Q; R3 = H, C1-4 alkyl; E = N, CH] and salts exert excellent aromatase-inhibitory activity in vivo and in vitro, with higher specificity and greater safety. Uses include treatment or prevention of a variety of estrogen-dependent diseases, and female contraception. For example, Ullmann-type etherification of 4-bromo-2-(1H-1,2,4-triazol-1-ylmethyl)phenol [preparation given] with 5-chloro-N-methyl-2-nitroaniline (62.5%), followed by Zn reduction of the nitro group, diazotization of the amine, cyclization to a benzotriazole (43% overall), and Pd-catalyzed cyanation of the bromide function (90%), gave title compound II. II inhibited rat ovarian aromatase in vitro and decreased blood estradiol in rats comparably to two known, similar compds., but unlike these compds. had no side effects on plasma aldosterone or 17α-hydroxyprogesterone levels.

IC ICM C07D233-60
ICS C07D249-08; C07D403-12; A61K031-41

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 2

ST azolylmethylphenyl naphthalene benzotriazole prepn aromatase inhibitor; estrogen dependent disease treatment aromatase inhibitor; triazole prepn aromatase inhibitor; imidazole prepn aromatase inhibitor

IT Neoplasm inhibitors
(preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)

IT Estrogens
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(treatment of related diseases; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)

IT Gynecomastia
Ovary, neoplasm
(treatment; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT Mammary gland
(disease, treatment; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT Mammary gland
(disease, benign, treatment; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT Prostate gland
(disease, benign hyperplasia, treatment; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT Puberty
(disorder, precocious, treatment; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT Parturition
(disorder, premature, treatment; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT Uterus, disease
(endometriosis, treatment; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT Uterus, neoplasm
(endometrium, treatment; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT Contraceptives
(female, preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT Uterus, neoplasm
(leiomyoma, treatment; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT Myoma
(leiomyoma, uterine, treatment; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT Fertility
(male, disorder, treatment; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT Mammary gland
(neoplasm, treatment; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT 52-39-1, Aldosterone 68-96-2, 17α-Hydroxyprogesterone
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(absence of effects on; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT 174265-21-5P
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT 50-28-2, Estradiol, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(effects on; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)
IT 2316-64-5P, 4-Bromo-2-(hydroxymethyl)phenol 2357-33-7P, 4-Fluoro-2-(hydroxymethyl)phenol 5330-38-1P, 4-Chloro-2-(hydroxymethyl)phenol 6341-99-7P, 2-Acetoxy-5-chlorotoluene 14056-07-6P, 2-(Hydroxymethyl)-4-iodophenol 35966-84-8P, 5-Chloro-N-methyl-2-nitroaniline 41951-76-2P, 2-(Hydroxymethyl)-4-methoxyphenol 60666-70-8P, 2-Bromo-5-chlorobenzyl alcohol 64917-81-3P,

5-Chloro-2-(hydroxymethyl)phenol 73671-65-5P 91827-44-0P, 4-Chloro-2-(hydroxymethyl)thiophenol 102806-77-9P, 2-Acetoxy-5-chlorobenzyl bromide 143218-46-6P, 5-Chloro-N-ethyl-2-nitroaniline 158979-33-0P, 2-(1H-1,2,4-Triazol-1-ylmethyl)phenol 162270-12-4P, 2-(Methoxymethoxy)-5-(trifluoromethyl)benzaldehyde 174264-53-0P, 1-(4-Chloro-2-methylphenoxy)naphthalene 174264-54-1P, 2-(4-Chloro-2-methylphenoxy)naphthalene 174264-55-2P, 1-[2-(Bromomethyl)-4-chlorophenoxy]naphthalene 174264-56-3P, 2-[2-(Bromomethyl)-4-chlorophenoxy]naphthalene 174264-60-9P, 5-Chloro-2-nitro-N-(trifluoroacetyl)aniline 174264-61-0P, 5-Chloro-N-methyl-2-nitro-N-(trifluoroacetyl)aniline 174264-62-1P, 2-(Hydroxymethyl)-4-(trifluoromethoxy)phenol 174264-63-2P 174264-64-3P 174264-65-4P 174264-66-5P 174264-67-6P 174264-68-7P 174264-69-8P 174264-70-1P 174264-71-2P 174264-72-3P 174264-73-4P 174264-74-5P 174264-75-6P 174264-76-7P 174264-77-8P 174264-78-9P 174264-79-0P 174264-81-4P 174265-01-1P, 2-(Methoxymethoxy)-5-(trifluoromethyl)benzyl alcohol 174265-02-2P, 2-(Hydroxymethyl)-4-(trifluoromethyl)phenol 174265-03-3P 174265-04-4P 174265-06-6P 174265-09-9P 174265-10-2P 174265-12-4P, 2-Bromo-5-chlorobenzaldehyde 174265-13-5P 174265-14-6P 174265-15-7P 174265-16-8P 174265-17-9P 174265-20-4P 174265-22-6P 174265-23-7P 174265-25-9P 174265-26-0P 174265-27-1P 174265-28-2P 174265-29-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)

IT 174264-82-5P 174264-85-8P 174264-86-9P **174264-94-9P** 174264-95-0P 174264-96-1P 174264-99-4P 174265-18-0P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)

IT 174264-57-4P 174264-58-5P 174264-59-6P 174264-80-3P 174264-83-6P 174264-84-7P 174264-87-0P 174264-88-1P 174264-89-2P 174264-90-5P 174264-91-6P 174264-92-7P 174264-93-8P 174264-97-2P 174264-98-3P 174265-00-0P 174265-05-5P 174265-07-7P 174265-08-8P 174265-11-3P **174265-19-1P**
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)

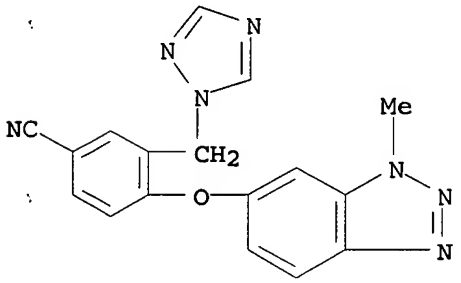
IT 9039-48-9, Aromatase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)

IT 64-18-6, Formic acid, reactions 75-36-5, Acetyl chloride 89-55-4, 5-Bromosalicylic acid 90-01-7, 2-(Hydroxymethyl)phenol 90-11-9, 1-Bromonaphthalene 288-32-4, Imidazole, reactions 288-88-0, 1H-1,2,4-Triazole 407-25-0, Trifluoroacetic anhydride 672-13-9, 5-Methoxysalicylaldehyde 1066-54-2, (Trimethylsilyl)acetylene 1570-64-5, 4-Chloro-2-methylphenol 1635-61-6, 5-Chloro-2-nitroaniline 1779-49-3, Methyltriphenylphosphonium bromide 5443-33-4, N-Acetyl-5-chloro-2-nitroaniline 14495-51-3, 2-Bromo-5-chlorotoluene 18162-48-6, t-Butylchlorodimethylsilane 93249-62-8, 5-(Trifluoromethoxy)salicylaldehyde 114408-87-6, 1-Methyl-1H-benzotriazole-

6-carboxaldehyde 120381-42-2, 5-Fluoro-N-methyl-2-nitroaniline 174265-24-8, 4-(Trifluoromethyl)phenyl methoxymethyl ether
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)

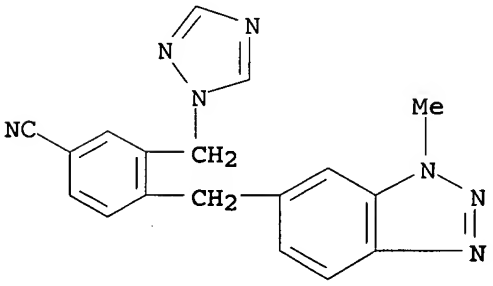
IT **174264-94-9P**
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)

RN 174264-94-9 HCAPLUS
CN Benzonitrile, 4-[(1-methyl-1H-benzotriazol-6-yl)oxy]-3-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)



IT **174265-19-1P**
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of (azolylmethyl)phenyl benzotriazoles and analogs as aromatase inhibitors)

RN 174265-19-1 HCAPLUS
CN Benzonitrile, 4-[(1-methyl-1H-benzotriazol-6-yl)methyl]-3-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

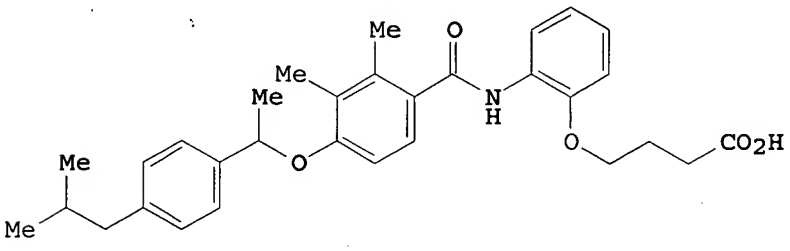


L54 ANSWER 15 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 1993:603668 HCAPLUS
DN 119:203668
TI Treatment of benign prostatic hyperplasia with a pharmaceutical combination of a 5α-reductase inhibitor and an aromatase inhibitor

IN Gormley, Glen J.; Stoner, Elizabeth
PA Merck and Co., Inc., USA
SO PCT Int. Appl., 289 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9218132	A1	19921029	WO 1992-US2749	19920406
	W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KR, LK, MG, MN, MW, NO, PL, RO, RU, SD				
	RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, MC, ML, MR, NL, SE, SN, TD, TG				
	AU 9218934	A	19921117	AU 1992-18934	19920406
	ZA 9202810	A	19921125	ZA 1992-2810	19920416
PRAI	US 1991-686720	A	19910417		
	US 1991-746388	A	19910816		
	US 1992-846155	A	19920311		
	WO 1992-US2749	A	19920406		

OS MARPAT 119:203668
GI



I

AB Combination therapy with a 5α-reductase inhibitor, e.g. a 4-azasteroid, a 17β-substituted non-azasteroid, a 17β-acyl-3-carboxyandrost-3,5-diene, a benzoylaminophenoxybutanoic acid, a cinnamoylamide, a fused benz(thio)amide, an aromatic 1,2-diether or thioether, an aromatic orthoacylaminophenoxyalkanoic acid, etc., and an aromatase inhibitor, e.g. fadrazole, is used for the treatment of benign prostatic hyperplasia (no data). Approx. 80 of the 5α-reductase inhibitors are prepared Tablets are prepared containing phenoxybutanoic acid I (preparation given).

IC ICM A61K031-58
ICS A61K045-06
ICI A61K031-58, A61K031-44
CC 32-4 (Steroids)
Section cross-reference(s): 1, 63
ST aromatase inhibitor reductase inhibitor prostatic hyperplasia; nonazasteroid fadrazole prostatic hyperplasia pharmaceutical
IT Prostate gland
(disease, hyperplasia, treatment of, with α-reductase inhibitor and aromatase inhibitor combination)
IT 9039-48-9D, Aromatase, mixture with α-reductase inhibitor
9081-34-9D, mixture with aromatase inhibitor
RL: USES (Uses)
(inhibitor, for treatment of prostatic hyperplasia)
IT 67963-68-2P 103335-48-4P **118634-65-4P**

RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

IT 65423-56-5P 73899-15-7P 87736-74-1P 139229-99-5P 144879-31-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for drug for treatment of benign prostatic hyperplasia)

IT 3903-40-0P 4082-57-9P 4560-41-2P 20012-63-9P 76763-14-9P
96692-02-3P 103335-41-7P 103335-44-0P 103335-47-3P 103335-49-5P
103335-50-8P 103335-54-2P 103335-55-3P 104239-97-6P 112290-15-0P
112290-16-1P 119169-84-5P 119347-93-2P 119347-94-3P 139229-98-4P
139230-00-5P 139230-01-6P 139230-02-7P 139230-03-8P 139230-04-9P
144879-11-8P 144879-12-9P 144879-14-1P 144879-15-2P 144879-16-3P
144879-17-4P 144879-18-5P 144879-22-1P 144879-23-2P 144879-24-3P
144879-28-7P 144879-30-1P 144879-42-5P 144879-43-6P 144879-44-7P
144879-45-8P 144879-46-9P 144879-47-0P 144879-49-2P 144879-50-5P
144879-54-9P 144879-55-0P 144879-58-3P 144879-59-4P 144879-60-7P
144879-61-8P 145191-60-2P 145191-61-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for drug for treatment of benign prostatic hypertrophy)

IT 98319-24-5P 98319-25-6P 98319-28-9P 98319-29-0P 103335-42-8P
103335-45-1P 103335-46-2P 103335-56-4P 103335-57-5P 103335-58-6P
103497-68-3P 119169-78-7P 119347-91-0P 119347-95-4P 119347-96-5P
119348-05-9P 119348-12-8P 133216-44-1P 133216-46-3P 134067-56-4P
134067-64-4P 134217-16-6P 134217-17-7P 138715-91-0P 139229-87-1P
139229-88-2P 139229-89-3P 139229-90-6P 139229-91-7P 139229-92-8P
139229-93-9P 139229-94-0P 139229-95-1P 139229-96-2P 139229-97-3P
139255-63-3P 139344-08-4P 139344-09-5P 139512-71-3P 139512-72-4P
139512-73-5P 139512-75-7P 139512-76-8P 139512-77-9P 139512-78-0P
139512-79-1P 139512-80-4P 139523-47-0P 139539-84-7P 139755-31-0P
144879-05-0P 144879-06-1P 144879-07-2P 144879-08-3P 144879-09-4P
144879-10-7P 144879-13-0P 144879-21-0P 144879-25-4P 144879-29-8P
144879-32-3P 144879-33-4P 144879-34-5P 144879-35-6P 144879-36-7P
144879-37-8P 144879-38-9P 144879-39-0P 144879-40-3P 144879-41-4P
144879-48-1P 148763-34-2P 148763-35-3P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, for use in combination therapy with aromatase inhibitors of benign prostatic hyperplasia)

IT 106-41-2, p-Bromophenol 15128-82-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of drug for treatment of benign prostatic hyperplasia)

IT 75-64-9, tert-Butylamine, reactions 88-75-5, 2-Nitrophenol 92-66-0, 4-Bromobiphenyl 100-39-0, Benzyl bromide 100-58-3 100-59-4, Phenylmagnesium chloride 104-92-7, p-Bromoanisole 104-95-0, p-Bromophenyl methyl sulfide 107-45-9, 2,4,4-Trimethyl-2-pentylamine 122-52-1, Triethyl phosphite 137-07-5, 2-Aminothiophenol 302-97-6 578-57-4, o-Bromoanisole 586-77-6, 4-Bromo-N,N-dimethylaniline 591-20-8, 3-Bromophenol 768-94-5, 1-Adamantanamine 873-75-6, 4-Bromobenzyl alcohol 931-51-1, Cyclohexylmagnesium chloride 2113-57-7, 3-Bromobiphenyl 2374-05-2, 4-Bromo-2,6-dimethylphenol 2635-13-4, 4-Bromo-1,2-methylenedioxybenzene 2834-05-1, 11-Bromoundecanoic acid 2969-81-5, Ethyl 4-bromobutyrate 4654-39-1, 2-(p-Bromophenyl)ethanol 5332-06-9, 4-Bromobutyronitrile 5674-02-2, Isobutylmagnesium chloride 6272-38-4, 2-Benzyloxyphenol 7242-92-4, exo-2-Aminonorbornane 10471-28-0, Diethyl 1,12-dodecanedioate 13074-39-0, 2-Adamantanamine 15366-08-2, sec-Butylmagnesium chloride 17768-41-1, Tricyclo[3.3.1.13,7]decane-1-methanamine 20607-43-6, Sodium isopropylthiolate 26825-95-6, Methyl 12-bromododecanoate 32916-51-1,

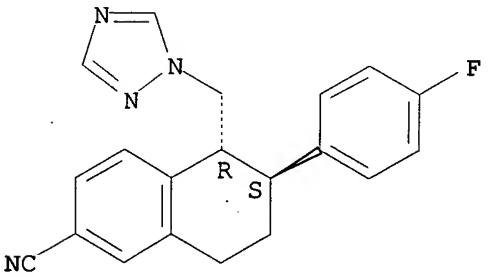
Cyclopentylmagnesium chloride 58380-40-8, 4-Hydroxy-2,3-dimethylbenzaldehyde 73367-80-3 73671-92-8 76124-42-0, Cyclobutylmagnesium chloride 86283-81-0 98319-26-7 103335-43-9 116751-23-6, 2-Pyrrolylmagnesium chloride 119347-92-1, 4-Isobutylbenzyl bromide 130387-74-5 146032-70-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of drug for treatment of benign prostatic hypertrophy)

IT 566-48-3 633-35-2, Androsta-1,4,6-triene-3,17-dione 5747-90-0 17781-31-6 26766-37-0 28217-83-6 35214-31-4 35214-35-8 68887-68-3, 1H-Imidazole-1-octanoic acid 76894-77-4 77016-85-4 91567-07-6 92788-10-8 96301-34-7 96400-02-1 102676-31-3 102676-47-1 102676-88-0 105051-72-7 105051-87-4 107868-30-4 112808-99-8 112809-51-5 112959-07-6 115575-11-6 118634-64-3 118634-66-5 118634-67-6 118635-00-0 118635-01-1 118635-05-5 118635-06-6 118635-15-7 118635-16-8 118635-17-9 118949-22-7 120319-52-0 120426-95-1 120427-12-5 120427-18-1 120427-25-0 120427-26-1 120427-32-9 120427-46-5 120456-91-9 120511-73-1 120511-93-5 120512-16-5 120512-55-2 120512-56-3 122023-37-4 122023-55-6 122023-56-7 122023-57-8 122023-66-9 122023-72-7 122266-46-0 123911-21-7 123911-51-3 123911-59-1 123911-81-9 129369-64-8 137555-33-0 137555-34-1 137555-35-2 137555-36-3 137578-72-4 137578-73-5 137624-20-5 137624-21-6 148665-04-7 148665-05-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(use of, with 5α-reductase inhibitors in combination therapy of benign prostatic hypertrophy)

IT **118634-65-4P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

RN 118634-65-4 HCAPLUS
CN 2-Naphthalenecarbonitrile, 6-(4-fluorophenyl)-5,6,7,8-tetrahydro-5-(1H-1,2,4-triazol-1-ylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



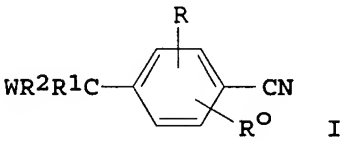
L54 ANSWER 16 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 1991:247287 HCAPLUS
DN 114:247287
TI Preparation and formulation of triazolylmethylbenzonitriles and analogs as aromatase inhibitors
IN Bowman, Robert M.; Steele, Ronald E.; Browne, Leslie
PA Ciba-Geigy Corp., USA
SO U.S., 19 pp. Cont.-in-part of U.S. 4,937,250.
CODEN: USXXAM
DT Patent
LA English

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4978672	A	19901218	US 1988-240862	19880906
	US 4749713	A	19880607	US 1986-837489	19860307
	US 4937250	A	19900626	US 1988-164696	19880307
	US 5112845	A	19920512	US 1990-628732	19901217
	US 5352795	A	19941004	US 1992-882188	19920511
	US 5473078	A	19951205	US 1994-275688	19940714
PRAI	US 1986-837489	A3	19860307		
	US 1988-164696	A2	19880307		
	US 1988-240862	A2	19880906		
	US 1990-628732	A3	19901217		
	US 1992-882188	A1	19920511		

OS MARPAT 114:247287

GI



I

AB The title compds. I [R, R° = H, alkyl; or R and R° located on adjacent carbon atoms and together when combined with the benzene ring to which they are attached form a naphthalene or tetrahydronaphthalene ring; R1, R2 = H, alkyl, alkenyl, cycloalkyl, etc.; W = (substituted) 1-imidazolyl, 1-(1,2,4- or 1,3,4)-triazolyl, 3-pyridyl] were prepared A mixture of α-bromo-p-tolunitrile, 1,2,4-triazole, K2CO3, and KI in acetone was stirred for 8 h at 55° to give I [R = R° = R1 = R2 = H; W = 1-(1,2,4-triazolyl)]. Compds. I exhibited IC50 values of 10-7 to 10-9 M against aromatase.

IC ICM A61K031-41
ICS C07D249-08

INCL 514383000

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

ST triazolylmethylbenzonitrile prepn aromatase inhibitor

IT Neoplasm inhibitors
((triazolylmethyl)benzonitriles and analogs)

IT Gynecomastia
((triazolylmethyl)benzonitriles effect)

IT Abortion
(by (triazolylmethyl)benzonitriles and analogs)

IT Estrogens
RL: RCT (Reactant); RACT (Reactant or reagent)
(inhibitors of biosynthesis of, (triazolylmethyl)benzonitriles as)

IT Contraceptives
(female, (triazolylmethyl)benzonitriles and analogs)

IT 9039-48-9, Aromatase
RL: USES (Uses)
(inhibitors, triazolylmethylbenzonitriles and analogs as)

IT 13391-47-4P 42252-33-5P 112808-96-5P 112809-49-1P 112809-50-4P
112809-58-2P 112809-59-3P 112809-60-6P 112809-61-7P 112809-62-8P
112809-63-9P 112809-64-0P 112809-65-1P 112809-69-5P 112809-70-8P
112809-71-9P 112809-73-1P 129696-66-8P 133982-02-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

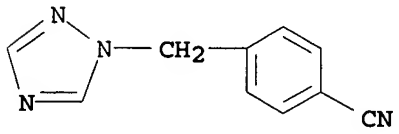
(Reactant or reagent)
(preparation and reaction of, in preparation of aromatase inhibitor)

IT 112808-94-3P 112808-96-5P 112808-98-7P 112808-99-8P 112809-00-4P
112809-01-5P 112809-03-7P 112809-05-9P 112809-06-0P 112809-07-1P
112809-08-2P 112809-09-3P 112809-11-7P 112809-12-8P 112809-13-9P
112809-14-0P 112809-15-1P 112809-16-2P 112809-17-3P 112809-18-4P
112809-19-5P 112809-20-8P 112809-21-9P 112809-22-0P 112809-23-1P
112809-24-2P **112809-25-3P 112809-26-4P** 112809-27-5P
112809-28-6P 112809-29-7P 112809-30-0P 112809-31-1P 112809-34-4P
112809-35-5P 112809-36-6P 112809-37-7P 112809-38-8P 112809-39-9P
112809-40-2P 112809-41-3P 112809-42-4P 112809-43-5P 112809-44-6P
112809-45-7P 112809-46-8P 112809-51-5P 112809-52-6P 112809-53-7P
112809-54-8P 112809-55-9P 112809-56-0P 112809-77-5P 112809-78-6P
129696-53-3P 129696-54-4P 129696-59-9P 129696-65-7P 133981-85-8P
133981-86-9P 133981-87-0P 133981-88-1P 133981-89-2P 133981-90-5P
133981-91-6P 133981-92-7P 133981-93-8P
133981-94-9P 133981-95-0P 133981-96-1P **133981-97-2P**
133981-98-3P 133981-99-4P 133982-00-0P 133982-01-1P
134000-92-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of, as aromatase inhibitor)

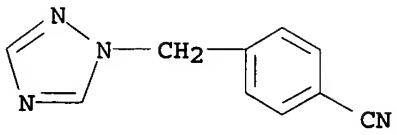
IT 90-96-0 104-88-1, 4-Chlorobenzaldehyde, reactions 288-32-4, Imidazole, reactions 288-88-0, 1H-1,2,4-Triazole 500-22-1, 3-Pyridinecarboxaldehyde 612-12-4 822-36-6, 4-Methylimidazole 874-86-2 1194-02-1, 4-Fluorobenzonitrile 10297-05-9 17201-43-3 42498-38-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of aromatase inhibitor)

IT **112809-25-3P 112809-26-4P 133981-91-6P**
133981-92-7P 133981-94-9P 133981-97-2P
134000-92-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of, as aromatase inhibitor)

RN 112809-25-3 HCAPLUS
CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

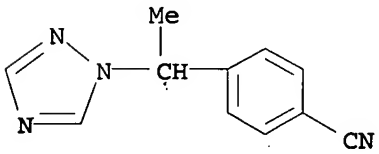


RN 112809-26-4 HCAPLUS
CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

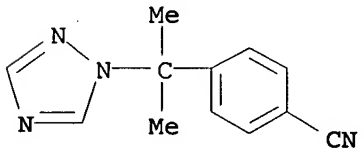


● HCl

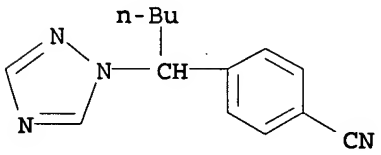
RN 133981-91-6 HCAPLUS
CN Benzonitrile, 4-[1-(1H-1,2,4-triazol-1-yl)ethyl]- (9CI) (CA INDEX NAME)



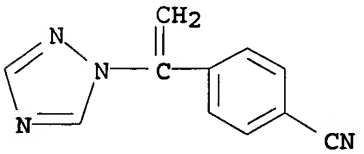
RN 133981-92-7 HCAPLUS
CN Benzonitrile, 4-[1-methyl-1-(1H-1,2,4-triazol-1-yl)ethyl]- (9CI) (CA INDEX NAME)



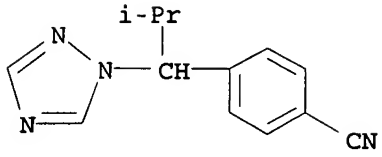
RN 133981-94-9 HCAPLUS
CN Benzonitrile, 4-[1-(1H-1,2,4-triazol-1-yl)pentyl]- (9CI) (CA INDEX NAME)



RN 133981-97-2 HCAPLUS
CN Benzonitrile, 4-[1-(1H-1,2,4-triazol-1-yl)ethenyl]- (9CI) (CA INDEX NAME)



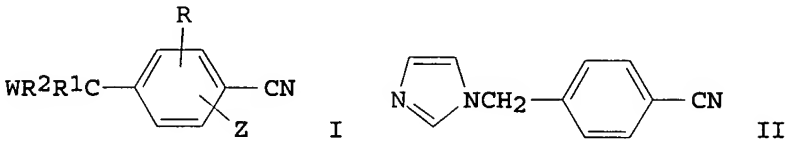
RN 134000-92-3 HCAPLUS
CN Benzonitrile, 4-[2-methyl-1-(1H-1,2,4-triazol-1-yl)propyl]- (9CI) (CA INDEX NAME)



L54 ANSWER 17 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 1990:631373 HCAPLUS
DN 113:231373
TI Preparation of (imidazolylmethyl)benzonitriles as aromatase inhibitors
IN Bowman, Robert M.; Steele, Ronald E.; Browne, Leslie J.
PA Ciba-Geigy Corp., USA
SO U.S., 16 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4937250	A	19900626	US 1988-164696	19880307
	US 4978672	A	19901218	US 1988-240862	19880906
	US 5071861	A	19911210	US 1990-510501	19900418
	US 5112845	A	19920512	US 1990-628732	19901217
	US 5352795	A	19941004	US 1992-882188	19920511
	US 5473078	A	19951205	US 1994-275688	19940714
PRAI	US 1986-837489	A3	19860307		
	US 1988-164696	A2	19880307		
	US 1988-240862	A2	19880906		
	US 1990-628732	A3	19901217		
	US 1992-882188	A1	19920511		

OS MARPAT 113:231373
GI



AB The title compds. I [R, Z = H, alkyl; or R and Z on adjacent C atoms and together when combined with the benzene ring to which they are attached form a naphthalene or tetrahydronaphthalene ring; R1 = H; R2 = aryl, arylalkyl, cyloalkyl, etc.; or R1R2 = alkylidene, mono-, diarylalkylidene, alkylene, etc.; W = (substituted) 1-imidazolyl; aryl = (substituted) Ph, 2-, 3-, or 4-pyridyl] were prepared A mixture of α-bromo-4-toluonitrile and imidazole in CH_2Cl_2 was stirred at room temperature for 15 h to give imidazole derivative II. II in vitro had an IC50 of 10 nM against aromatase.
IC ICM A61K031-415
ICS C07D401-06
INCL 514341000
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
ST imidazolylmethylbenzonitrile prepn aromatase inhibitor; benzonitrile

imidazolylmethyl prepn aromatase inhibitor

IT Gynecomastia
((imidazolylmethyl)benzonitriles effect on)

IT Estrogens
RL: RCT (Reactant); RACT (Reactant or reagent)
(inhibitors of biosynthesis of, (imidazolylmethyl)benzonitriles as)

IT Parturition
(disorder, premature, (imidazolylmethyl)benzonitriles effect on)

IT Uterus, disease or disorder
(endometriosis, treatment of, (imidazolylmethyl)benzonitriles for)

IT 9039-48-9, Aromatase
RL: RCT (Reactant); RACT (Reactant or reagent)
(inhibitors of, (imidazolylmethyl)benzonitriles as)

IT 13428-06-3P 42252-33-5P 112809-57-1P 112809-58-2P 112809-59-3P
112809-60-6P 112809-61-7P 112809-62-8P 112809-63-9P 112809-64-0P
112809-65-1P 112809-66-2P 112809-69-5P 129696-66-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of aromatase inhibitor)

IT 129696-68-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

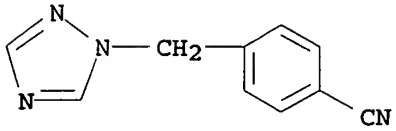
IT 112808-94-3P 112808-96-5P 112808-99-8P 112809-00-4P 112809-01-5P
112809-02-6P 112809-03-7P 112809-05-9P 112809-06-0P 112809-07-1P
112809-08-2P 112809-09-3P 112809-10-6P 112809-11-7P 112809-12-8P
112809-13-9P 112809-14-0P 112809-15-1P 112809-16-2P 112809-17-3P
112809-18-4P 112809-19-5P 112809-20-8P 112809-21-9P 112809-22-0P
112809-23-1P 112809-24-2P **112809-25-3P 112809-26-4P**
112809-27-5P 112809-28-6P 112809-29-7P 112809-30-0P 112809-31-1P
112809-31-1P 112809-35-5P 112809-36-6P 112809-37-7P 112809-38-8P
112809-39-9P 112809-42-4P 112809-43-5P 112809-44-6P 112809-46-8P
112809-47-9P 112809-48-0P 112809-49-1P 112809-50-4P 112809-51-5P
112809-52-6P 112809-54-8P 112809-55-9P 112809-56-0P 112809-71-9P
112809-75-3P 112809-77-5P 112809-78-6P 129696-53-3P 129696-54-4P
129696-55-5P 129696-57-7P 129696-58-8P 129696-59-9P 129696-60-2P
129696-61-3P 129696-62-4P 129696-63-5P 129696-64-6P 129696-65-7P
129696-67-9P 129717-95-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of, as aromatase inhibitor)

IT 74-88-4, reactions 79-44-7, N,N-Dimethylcarbamoyl chloride 90-96-0, 4,4'-Dimethoxybenzophenone 104-88-1, 4-Chlorobenzaldehyde, reactions 109-94-4 288-32-4, 1H-Imidazole, reactions 288-88-0, 1H-1,2,4-Triazole 612-12-4, α,α'-Dichloro-o-xylene 822-36-6 882-33-7 1194-02-1, 4-Fluorobenzonitrile 10297-05-9, 1-Chloro-4-iodobutane 17201-43-3 30525-89-4, Paraformaldehyde 42498-38-4 112809-74-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of aromatase inhibitor)

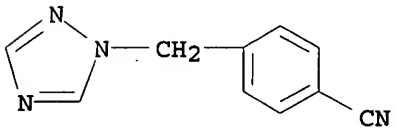
IT **112809-25-3P 112809-26-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of, as aromatase inhibitor)

RN 112809-25-3 HCAPLUS

CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)



RN 112809-26-4 HCAPLUS
CN Benzonitrile, 4-(1H-1,2,4-triazol-1-ylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

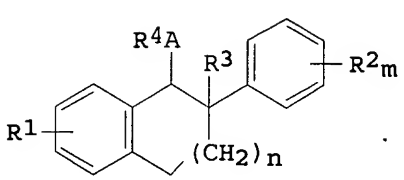


○ HCl

L54 ANSWER 18 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:75517 HCAPLUS
DN 110:75517
TI Preparation of nitrogen-containing heterocycles as aromatase inhibitors
IN Boyle, Francis Thomas; Matusiak, Zbigniew Stanley; Tait, Brian Steele
PA Imperial Chemical Industries PLC, UK
SO Eur. Pat. Appl., 20 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 281283	A1	19880907	EP 1988-301399	19880219
	EP 281283	B1	19930210		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	ZA 8801008	A	19881026	ZA 1988-1008	19880212
	US 4910212	A	19900320	US 1988-155803	19880216
	AU 8811934	A	19880908	AU 1988-11934	19880218
	AU 612623	B2	19910718		
	AT 85613	T	19930215	AT 1988-301399	19880219
	DK 8801126	A	19880906	DK 1988-1126	19880302
	CA 1304741	C	19920707	CA 1988-560397	19880303
	FI 8801018	A	19880906	FI 1988-1018	19880304
	NO 8800987	A	19880906	NO 1988-987	19880304
	NO 169894	B	19920511		
	NO 169894	C	19920819		
	JP 63238070	A	19881004	JP 1988-49947	19880304
PRAI	GB 1987-5174	A	19870305		
	EP 1988-301399	A	19880219		

OS MARPAT 110:75517
GI



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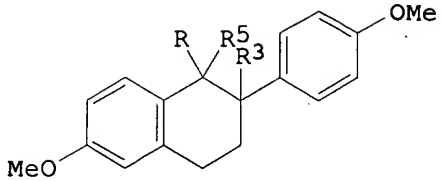


IV

AB Title compds. I [R1, R2 = H, halo, (mono- or dialkyl-substituted) amino, (mono- or dialkyl-substituted)carbamoyl, cyano, OH, (mono- or dialkyl-substituted)sulfamoyl, NO2, haloalkyl, alkyl, alkoxy, haloalkoxy, alkoxycarbonyl; R3 = H, halo, alkyl, haloalkyl; R4 = 5-membered aromatic heterocyclyl containing 2 or 3N, 6-membered aromatic heterocyclyl containing 1 or 2N;
m = 1-5; n = 0, 1; A = (alkyl-substituted) C1-4 alkylene] (II) useful as aromatase inhibitors and anticancer agents (no data) are prepared from I (R4 = leaving group) (III) and R4H. Treatment of naphthalene IV (R = CHO; R3R5 = bond) (preparation given) with LiAlH4 in Et2O gave IV (R = CH2OH), which in AcOEt was hydrogenated in the presence of 10% Pd/C to afford IV (R = CH2OH; R3 = R5 = H), and a solution of the latter alc. and Et3N in CH2Cl2 was stirred with MeSO2Cl to give IV (R = CH2OSO2Me; R3 = R5 = H) (V). A solution of (1R,2R)-V, imidazole, and K2CO3 in MeCN was refluxed to yield (1R,2R)-IV (R = 1-imidazolylmethyl; R3 = R5 = H).

IC ICM C07D249-08
ICS C07D233-64; C07D213-06; C07D237-08; C07D239-08; A61K031-41

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST heterocycle nitrogen contg aromatase inhibitor

IT 9039-48-9, Aromatase
RL: USES (Uses)
(inhibitors, nitrogen-containing heterocycles as)

IT 118601-96-0P 118601-97-1P 118601-98-2P 118601-99-3P 118602-00-9P
118602-01-0P 118602-02-1P 118602-03-2P 118602-04-3P 118602-05-4P
118602-06-5P 118602-07-6P 118602-08-7P 118602-09-8P 118602-10-1P
118602-11-2P 118602-12-3P 118602-13-4P 118602-14-5P 118602-15-6P
118602-16-7P 118602-17-8P 118602-18-9P 118602-19-0P 118602-20-3P
118602-21-4P 118602-22-5P 118602-23-6P 118602-25-8P 118602-26-9P
118602-27-0P 118602-32-7P 118602-33-8P 118602-34-9P 118602-35-0P
118602-36-1P 118602-37-2P 118602-38-3P 118634-61-0P 118634-62-1P
118711-40-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of aromatase inhibitors)

IT 118602-39-4P 118634-63-2P **118634-64-3P** **118634-65-4P**
118634-66-5P 118634-67-6P 118634-68-7P 118634-69-8P
118634-70-1P 118634-71-2P **118634-72-3P** 118634-73-4P
118634-74-5P 118634-75-6P 118634-76-7P 118634-77-8P 118634-78-9P
118634-79-0P 118634-80-3P 118634-81-4P 118634-82-5P 118634-83-6P
118634-84-7P 118634-85-8P 118634-86-9P 118634-87-0P 118634-88-1P
118634-89-2P 118634-90-5P 118634-91-6P 118634-92-7P 118634-93-8P
118634-94-9P 118634-95-0P 118634-96-1P 118634-97-2P 118634-98-3P
118634-99-4P 118635-00-0P 118635-01-1P 118635-02-2P 118635-03-3P
118635-04-4P 118635-05-5P 118635-06-6P 118635-07-7P 118635-15-7P
118635-16-8P **118635-17-9P** 118687-82-4P 120938-73-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)

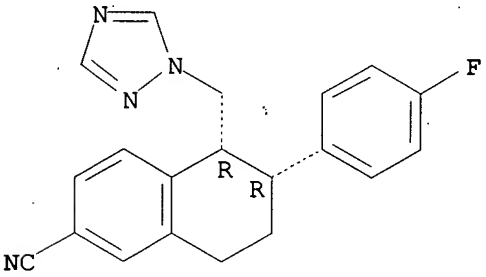
(preparation of, as aromatase inhibitor)

IT 105-36-2, Ethyl bromoacetate 288-32-4, Imidazole, reactions 288-88-0, 1H-1,2,4-Triazole 822-36-6, 4-Methylimidazole 4009-98-7 5459-40-5, 4-Ethoxystyrene 7677-24-9, Trimethylsilylcarbonitrile 56437-05-9 82594-80-7, 1-Trityl-4-methylimidazole 96034-06-9 96034-07-0 118602-24-7 118602-28-1 118602-29-2 118602-30-5, 6-Bromo-2-(4-fluorophenyl)tetralone 118602-31-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of aromatase inhibitors)

IT **118634-64-3P 118634-65-4P 118634-70-1P 118634-72-3P 118635-16-8P 118635-17-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of, as aromatase inhibitor)

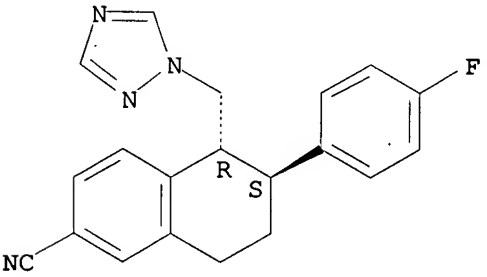
RN 118634-64-3 HCAPLUS
CN 2-Naphthalenecarbonitrile, 6-(4-fluorophenyl)-5,6,7,8-tetrahydro-5-(1H-1,2,4-triazol-1-ylmethyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



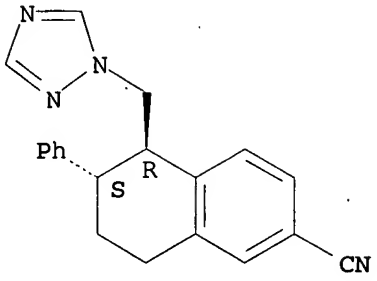
RN 118634-65-4 HCAPLUS
CN 2-Naphthalenecarbonitrile, 6-(4-fluorophenyl)-5,6,7,8-tetrahydro-5-(1H-1,2,4-triazol-1-ylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



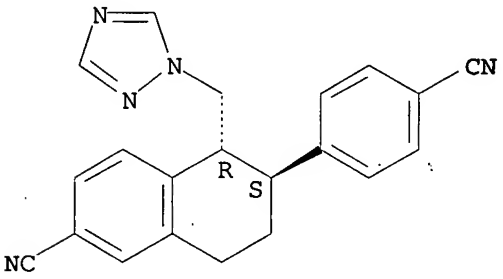
RN 118634-70-1 HCAPLUS
CN 2-Naphthalenecarbonitrile, 5,6,7,8-tetrahydro-6-phenyl-5-(1H-1,2,4-triazol-1-ylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



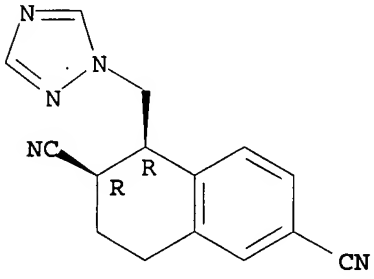
RN 118634-72-3 HCAPLUS
CN 2-Naphthalenecarbonitrile, 6-(4-cyanophenyl)-5,6,7,8-tetrahydro-5-(1H-1,2,4-triazol-1-ylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



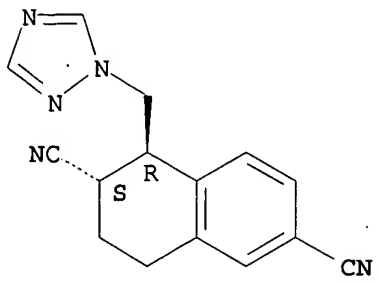
RN 118635-16-8 HCAPLUS
CN 2,6-Naphthalenedicarbonitrile, 1,2,3,4-tetrahydro-1-(1H-1,2,4-triazol-1-ylmethyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 118635-17-9 HCAPLUS
CN 2,6-Naphthalenedicarbonitrile, 1,2,3,4-tetrahydro-1-(1H-1,2,4-triazol-1-ylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.


N
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